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Whitepaper

The Challenges in Modeling and Simulation of Fluoride-Salt-Cooled High-Temperature Reactors

Prepared by F. Rahnema[1], B. Petrovic[1], P. Singh[1], P. Burke[1], H. Noorani[1], X. Sun[2], G. Yoder[3], P. Tsvetkov[4], J. Zhang[5], D. Zhang[1], D. Ilas[3]

[1] Georgia Institute of Technology, [2] University of Michigan, [3] Oak Ridge National Lab, [4] Texas A&M University, [5] Virginia Polytechnic Institute and State University

Computational Reactor and Medical Physics Laboratory
Nuclear and Radiological Engineering Programs
Georgia Institute of Technology
Atlanta, GA 30332

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Executive Summary

Accurate modeling and simulation (M&S) methods and tools are necessary to support design, analysis, and licensing of any reactor. This is one of the challenges that must be addressed for deployment of fluoride-salt-cooled high-temperature reactors (FHRs), as current M&S tools are insufficient due to unique phenomena associated with FHR operation including multiple heterogeneity in the reactor core, potentially large uncertainties in some of the fundamental cross section data for key reactor components, and others.

FHRs offer benefits that include improved safety, proliferation-resistant waste, and improved thermodynamic efficiency due to higher operating temperatures. However, before these reactors can be deployed, several key technologies need to be developed further. In 2015, the U.S. Department of Energy initiated two university-led Integrated Research Projects (IRP) to address challenges associated with several of these technologies, one led by Georgia Tech (GT), and one led by the Massachusetts Institute of Technology (MIT). To address the M&S challenge, the GT-led IRP organized several PIRT exercises to identify fundamental, underlying issues with FHR modeling. Additionally, the two IRP teams jointly organized an FHR M&S Workshop to identify gaps in current M&S tools.

To begin identifying and categorizing these issues, four Phenomena Identification and Ranking Tables (PIRT) exercises were organized (one each for neutronics, thermal-hydraulics, materials, and multiphysics) by the GT-led IRP team, with panels consisting of experts from academia, national labs, and industry. The reports produced by these PIRT exercises enumerate fundamental, underlying challenges to FHR modeling that are not specific to any one tool. The only PIRT results presented in this document are those phenomena identified as being of high or medium importance, with a low level of knowledge on the subject.

For the neutronics PIRT exercise, phenomena were categorized into four areas: fundamental cross section data, material composition, computational methodology, and general depletion. Cross section data included phenomena such as moderation in FLiBe, thermalization in FLiBe, and others. Material composition included only one phenomenon: fuel particle distribution of TRISO particles in real fabricated fuel. Computational Methodology included phenomena such as: solution convergence, granularity of depletion regions, multiple heterogeneity treatment, and others. The only phenomenon related to general depletion is that of spectral history effects.

The thermal-hydraulics (T/H) PIRT exercise began by identifying a list of accident scenarios considered to be of paramount importance in FHR licensing. Two scenarios were selected for focus with detailed discussion: station blackout, and simultaneous withdrawal of control rods. Within these scenarios, thirteen and twelve phenomena, respectively, were identified as needing further study to understand and accurately model the accident. These phenomena included thermal conductivity of FLiBe, wall friction in the core, core flow asymmetry, and others.

The materials PIRT report is very detailed, and identifies phenomena relating to salt interaction with many different materials in the context of six structural applications: vessel and primary piping, primary heat exchanger, steam generator tubes and vessel, intermediate loop piping, valves and pumps, and welds. Within each relevant material/application combination, phenomena are identified, including cladding interdiffusion, cladding delamination, creep, and others.

The multiphysics PIRT panel examined three scenarios: Normal Operation, Station Blackout, and Simultaneous Withdrawal of All Control Rods. Additionally, another category was created for phenomena that didn't fall under one of these scenarios. Within these categories, phenomena were identified as requiring "tight" coupling (involving detailed iterative feedback between two codes/models) or "loose" coupling (involving sharing of precalculated information). The phenomena requiring "tight" coupling are presented in this document. These included the energy generation rate in fuel kernel, upper plenum mixing, heat transfer to fusible links, and others.

To discuss code-level gaps and modeling challenges, an FHR M&S Workshop was held at Georgia Tech on March 8-9, 2017, jointly organized by Georgia Tech, MIT, and UCB. Building off the knowledge produced in the PIRT exercises, this workshop reviewed the capabilities of the current tools for analysis of FHRs, and identified the gaps and needs for the development, extension, and/or V&V of existing tools necessary to support the licensing of FHRs. At the workshop, three breakout sessions (one each for neutronics, thermal-hydraulics, and materials) were held to discuss modeling challenges, needs, and gaps in that area.

The neutronics breakout session first discussed the issue of prohibitively large computation time with full-scale, full-detail FHR modeling for both stochastic and deterministic methods. The discussion then continued to the applicability of SCALE and the NEAMS ToolKit to FHR – tools of particular interest to the GT-led IRP. The result of the SCALE discussion was that its capabilities with respect to the multiple heterogeneity of the studied FHR designs, as well as the result of spectral effects on cross section generation, need to be studied. The NEAMS discussion concluded that, for it to be a complete toolkit, it needs to include a stochastic module for reference solution generation (the idea of SHIFT integration was mentioned). Additionally, the planned mesh-based interface would prove very useful. A large list[1] of modeling issues that are not code-specific was then created, with some of the most important points being multi-group cross section generation to account for multiple heterogeneity, development of an appropriate and optimized multi-group structure, and gaps in current core transient calculation capabilities.

The thermal-hydraulics breakout session began by defining a context of discussion, including a list of reactor operation scenarios that need to be modeled, and a list of codes

[1] Not included here, for brevity. Can be found in full document

and methodologies to be discussed. In this context, three broad categories of modeling and simulation issues were discussed: broad T/H M&S challenges, gaps in current data libraries, and gaps in current codes pertaining to modeling FHR-specific phenomena. Broad challenges included the computational cost associated with full-scale, full-detail modeling; the fact that many of the required scenarios/initiating events require multiphysics modeling due to effects such as salt freezing; the lack of tools that can simulate dynamic system response at a level that includes the power conversion system; and a lack of understanding about uncertainty analysis for certain T/H experiments and calculations as they relate to thermo-physical properties. The gaps in current data libraries include thermo-physical properties of salts (thermal conductivity, viscosity, IR absorption, etc.), thermal conductivity and heat capacity of structural materials over a broad temperature range, and heat transfer coefficients and wall friction coefficients for different FHR fuel types. The list of gaps relating to FHR-specific phenomena is not printed here for brevity, but can be found in the full document.

The materials breakout session began by acknowledging that there is very little M&S activity surrounding corrosion or degradation of structural materials in molten salts, as most existing codes (e.g., MOOSE and BISON) focus on fuel simulation with little to no applicability for structural simulations. Next, implementation possibilities in this area were discussed, including the adaptation of thermodynamic models for corrosion predictions, the coupling of lower-level physics codes (e.g., a molecular dynamics code) and upper-level effects codes, and coupling materials and computational fluid dynamics (CFD) codes to investigate the effect of flowing and stagnant coolant zones. It was then acknowledged that uncertainty in the effect of carbon contamination of coolant salts could cause a large difference between structural material model predictions and practical application. Like in the other breakout sessions, the need for validated experimental data was underscored. Specifically, the need for standardized ways to measure redox of FHR molten salts was discussed, such that the results from different experimental studies under different conditions can be compared. Additionally, it was mentioned that there is a need for cost-effective alternatives to expensive in-core experiments, such as near-core or simulated radiolysis chemistry loops. There was also a concern with the lack of data on the effect of radiation on selected structural materials. These materials will need to be code approved for use in construction, so data needs to be collected on corrosion of joints, welds, laminated structures, etc. It was emphasized that there is a need to coordinate with neutronics code developers to create a feedback system to capture phenomena such as the effect of tritium production. Finally, it was underscored that some required thermodynamic data is not available, and a coordinated effort is required to generate and validate this data, which is needed to model and simulate corrosion processes in FHR.

It is clear from these exercises that there is profound interest in this research area. The underlying conclusion from the PIRT panels, workshop, and thus this whitepaper, is that there is a number of gaps in current tools for FHR modeling and simulation. For use in design, analysis, and licensing of an FHR, the important gaps must be closed. *It is demonstrated by the PIRT exercises and the workshop discussion that a broader organized push is needed to develop, verify, and validate these capabilities.*

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List of Abbreviations

AHTR	Advanced High Temperature Reactor	MIT	Massachusetts Institute of Technology
ANL	Argonne National Laboratory	MSR	Molten Salt Reactor
ATWS	Anticipated Transients with Scram	MWe	Megawatt-electric
C-C	Carbon-Carbon	NACC	Nuclear Air-Brayton Combined Cycle
CE	Continuous Energy	NDHX	Natural Draft Heat Exchanger
CFD	Computational Fluid Dynamics	NRC	Nuclear Regulatory Commission
CSP	Concentrated Solar Power	ORNL	Oak Ridge National Lab
DHX	Direct Heat Exchanger	PB-FHR	Pebble-Bed FHR
DRACS	Direct Reactor Auxiliary Control System	PIRT	Phenomena Identification and Ranking Tables
EMI	Electromagnetic Interference	RSICC	Radiation Safety Information Computation Center
FHR	Fluoride-salt-cooled High-temperature Reactors	SINAP	Shanghai Institute of Applied Physics
GT	Georgia Institute of Technology	T/H	Thermal-hydraulics
GUI	Graphical User Interface	TAMU	Texas A&M University
HTGR	High Temperature Gas Reactor	TRISO	Tristructural-isotropic
IRP	Integrated Research Project	UCB	University of California at Berkeley
JEFF	Joint Evaluated Fission and Fusion File	U-Mich	University of Michigan
LOCA	Loss of Coolant Accident	UNM	University of New Mexico
LOOP	Loss of Offsite Power	USDOE	U.S. Department of Energy
LWR	Light Water Reactor	UW	University of Wisconsin at Madison
M&S	Modeling and Simulation	V&V	Verification and Validation
MG	Multi-group	VHTR	Very High Temperature Reactor
MHD	Magnetohydrodynamics	VT	Virginia Tech

Introduction

Fluoride-cooled High-temperature Reactor (FHR) designs offer benefits that include the promise of improved safety, proliferation-resistant waste, and improved thermodynamic efficiency due to higher operating temperatures. Deployment of this technology would expand the role of nuclear power in the modern energy marketplace, as well as allow it to meet the future demand for industrial process heat. Recently, the U.S. Department of Energy initiated two university-led Integrated Research Projects (IRP) to address challenges associated with several of these technologies.

The Georgia Institute of Technology is leading a team of researchers with major collaborators from Texas A&M University (TAMU), Texas A&M University Kingsville (TAMU-K), University of Michigan (U-Mich), Virginia Tech (VT), Oak Ridge National Laboratory (ORNL), and AREVA, as well as international partners at University of Zagreb, Politecnico di Milano, and Shanghai Institute of Applied Physics (SINAP). The GT led IRP chose the ORNL preconceptual design for the Advance High Temperature Reactor (AHTR) as its reference design for analysis and technology development. The Massachusetts Institute of Technology (MIT) is leading another team of researchers from the University of California at Berkeley (UCB), University of New Mexico (UNM), and the University of Wisconsin at Madison (UW). This team chose the Mark 1 Pebble-Bed FHR (MK1 PB-FHR) pre-conceptual design as their reference reactor for their technology development and analysis.

There is an increased demand for comprehensive modeling and simulation (M&S) tools for design, safety analysis, and operation in support of licensing of these reactors. These tools can also be used to design experiments. Current FHR conceptual designs pose unique challenges to existing tools. To address these challenges, new modules/methodologies may be required and/or existing codes may need to be adapted.

To begin identifying and categorizing these capability gaps, four Phenomena Identification and Ranking Tables (PIRT) exercises were organized by the GT-led IRP team, with panels consisting of experts from academia, national labs, and industry. The reports produced by these PIRT exercises enumerate fundamental, underlying challenges to FHR modeling that are not specific to any one code.

To build on the knowledge produced during those PIRT exercises, Georgia Tech together with MIT and UCB jointly organized an FHR M&S workshop, held at Georgia Tech on March 8-9, 2017. Attendees included members of academia, the U.S.D.O.E. and N.R.C., National Lab Employees, and others. This workshop had three main purposes:

- Give M&S code developers and experts the opportunity to discuss their code and its relative applicability to FHRs
- Create a forum, through research area-specific breakout sessions, where these code developers could collaborate with their users to identify code-specific gaps in FHR modeling
- Discuss these modeling challenges and gaps, and identify a path forward.

This whitepaper serves as a summary of the results of these exercises and, in doing so, characterizes the current state of FHR M&S capabilities. It contains:

1. An overview of the reference designs being considered by the two FHR-IRP teams. These are provided as an example of reactor designs that any comprehensive M&S tool must be able to model with desired accuracy.
2. An overview of several codes discussed in the workshop. These are intended to provide a reader unfamiliar with a specific code a brief description of its current capability, as well as past application to FHR.
3. A summary of the PIRT exercises performed by the GT-led IRP team. These summaries discuss fundamental, underlying modeling issues and challenges that are unique to FHR designs.
4. An overview of the FHR M&S workshop held at Georgia Tech on March 8-9, 2017. The agenda for the event as well as the attendee list are provided to give the reader with an idea of how the workshop was conducted.
5. A summary of the results of the breakout sessions at the FHR M&S workshop. The issues identified here are largely code-level gaps and challenges identified by both researchers and code experts.
6. A few overarching conclusions about the results of the PIRT exercises and the workshop discussion.

This document then concludes with remarks about the path forward for FHR M&S.

1. AHTR & PB-FHR Reactor Overview

This section contains a brief overview of the reference reactors being analyzed by the two FHR-IRP teams: the AHTR and the MK1 PB-FHR. This section contains only a brief description of the important features of the reactors that pose unique challenges to modeling and simulation. These descriptions are provided for use as a reference for readers to assess the capabilities of their code with respect to modeling these reactors.

All information and figures for the AHTR summary come directly from the ORNL document "AHTR Mechanical, Structural, and Neutronic Preconceptual Design" by Varma et al. (2012). All information and figures for the PB-FHR summary come directly from the UCB document "Technical Description of the "Mark 1" Pebble-Bed Fluoride-Salt-Cooled High-Temperature Reactor (PB-FHR) Power Plant" by Andreades et al. (2012). For a more detailed description of the AHTR or the PB-FHR, see these documents.

A simplified numerical description of the AHTR is under development for of numerical verification of neutronics methods.

1.1. AHTR Reactor Overview

The FHR-IRPs are working with two different pre-conceptual designs for an FHR. The team led by Georgia Tech is working with the Advanced High-Temperature Reactor developed at Oak Ridge National Lab to "enable evaluation of the technology hurdles remaining to be overcome prior to FHRs becoming an option for commercial reactor deployment."

The AHTR is a design concept for a 3400 MWth FHR. An overview of the reactor cooling systems can be seen in Figure 1. The salt in the primary coolant loop is a mixture of LiF (enriched to 99.995% ^{7}Li) and BeF_2 (FLiBe). The salt in the intermediate loop and DRACS is a KF-ZrF4 salt, and transfers heat to a supercritical steam power cycle.

The core, seen in Figure 2, is a hexagonal array of 252 fuel assemblies. The assemblies are loaded with a two-batch loading scheme. The core includes replaceable reflectors on the periphery of the core, in addition to the permanent reflector.

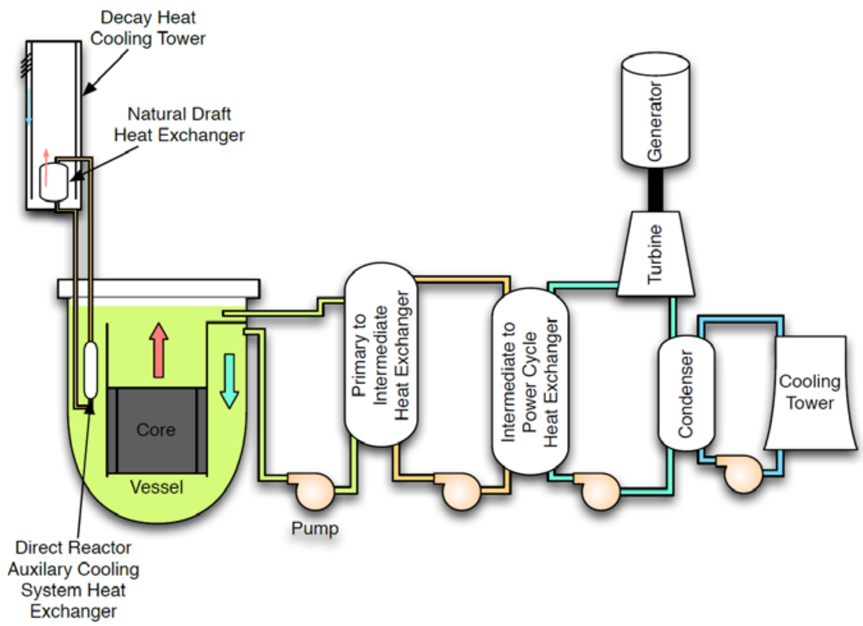

Figure 1 – AHTR Systems Overview

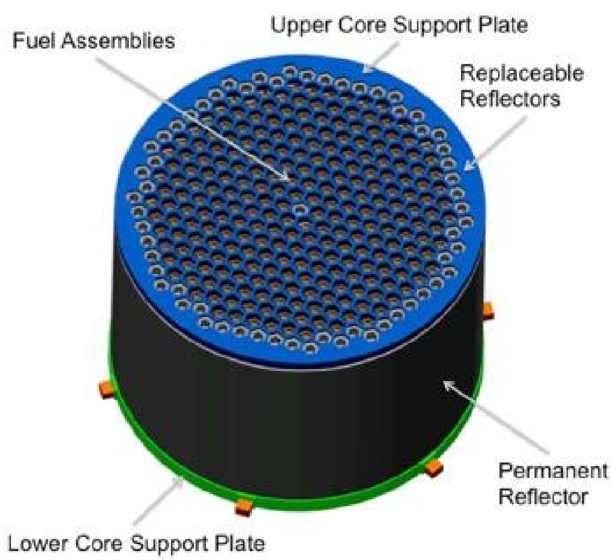

Figure 2 – AHTR Core

The assemblies, seen in Figure 3, are hexagonal prisms with 18 fuel plates. The fuel plates are enclosed in a Carbon-Carbon (C-C) composite fuel box and inner support structure. The inner C-C support also includes a Y-shaped gap to allow for insertion of the molybdenum hafnium carbide control blade. Surrounding each plate, there are coolant flow channels, maintained by spacer ridges on the outer graphite sleeve of the plate.

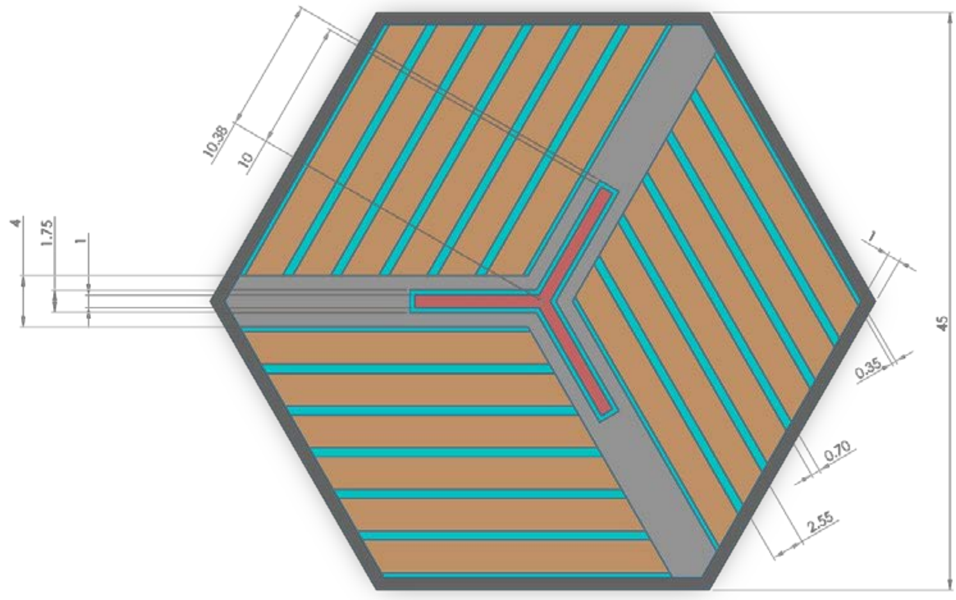

Figure 3 – AHTR Assembly Cross Section (Huang, Avigni, & Petrovic, 2015)

The fuel plate, shown in Figure 4, consists of tristructural isotropic (TRISO) fuel particles suspended in a high-density graphite matrix. The TRISO particles are pressed into two fuel stripes, one on each side of the plate. BISO burnable poison particles may be used in the center of the plate for fresh core reactivity control. As mentioned above, there are also spacer ridges in the outer graphite that maintain the separation between plates to allow for coolant flow.

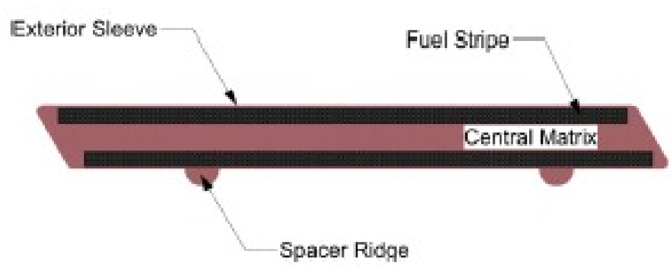

Figure 4 – AHTR Fuel Plate

The TRISO fuel particles, shown in Figure 5, consist of a fuel kernel encapsulated by four other layers: an outer pyrocarbon layer, silicon carbide layer, an inner pyrocarbon layer, and a less dense carbon buffer layer. TRISO fuel is being explored for many advanced reactor concepts.

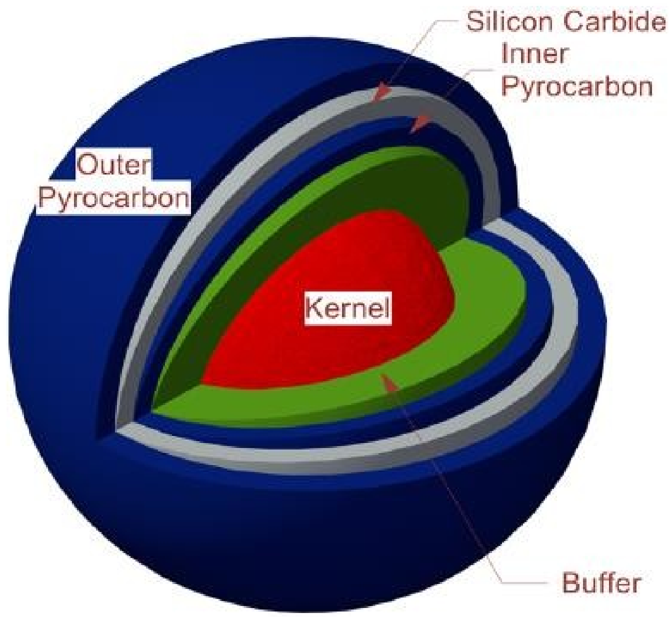

Figure 5 – TRISO Fuel Particle

1.2. MK1 PB-FHR Overview

The MK1 Pebble-Bed Fluoride-cooled High-temperature Reactor (PB-FHR) is a pre-conceptual design for a small modular 236 MWth FHR. This design also features the use of a nuclear air-Brayton combined cycle (NACC) that enables natural gas co-firing. This enables the 100 MWe nuclear-only generation to be boosted up to 242 MWe by natural gas. This allows the PB-FHR to better match the landscape of the future energy market by allowing for synergy with variable capacity sources like wind and solar. An overview of these systems can be seen in Figure 6. Note, the color of the arrows in the diagram corresponds to the working fluid.

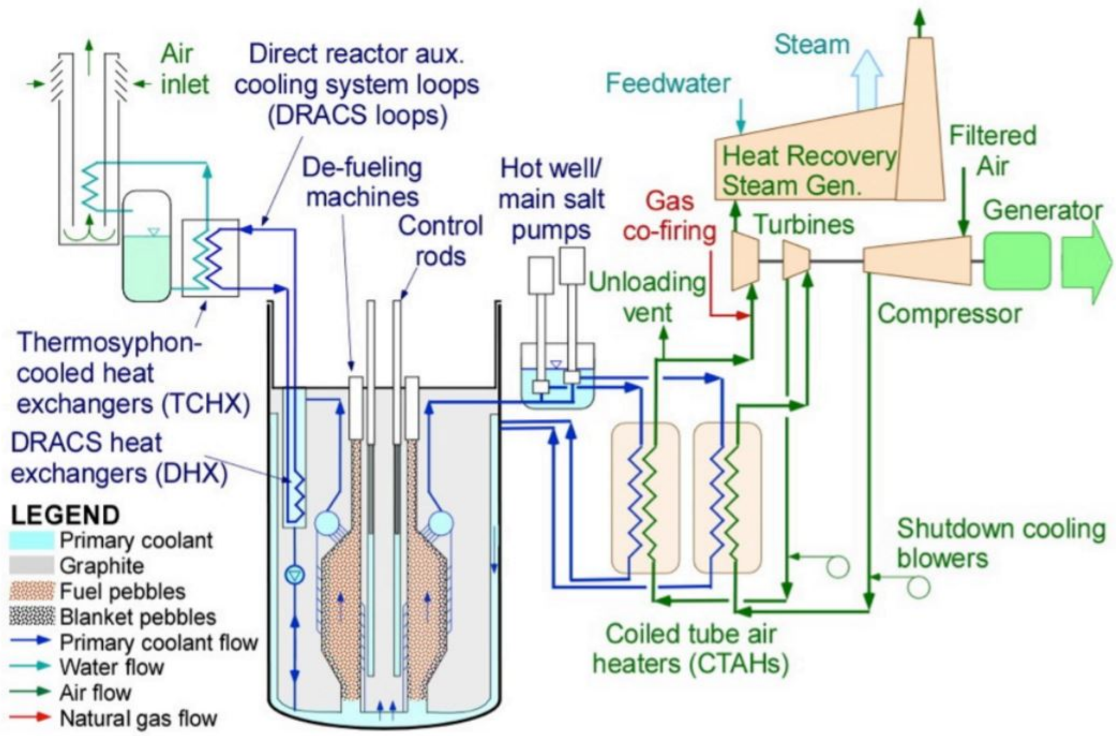

Figure 6 – PB-FHR Plant Overview

The core, seen in Figure 7, consists of an annulus of fuel pebbles and blanket pebbles. Because the less-dense fuel pebbles float in the dense FLiBe coolant, pebbles are injected in the bottom of the bed. The pebbles travel up through the core and are removed by one of two defueling machines at the top of the core. The average in-core residence time of one pebble is 2.1 months.

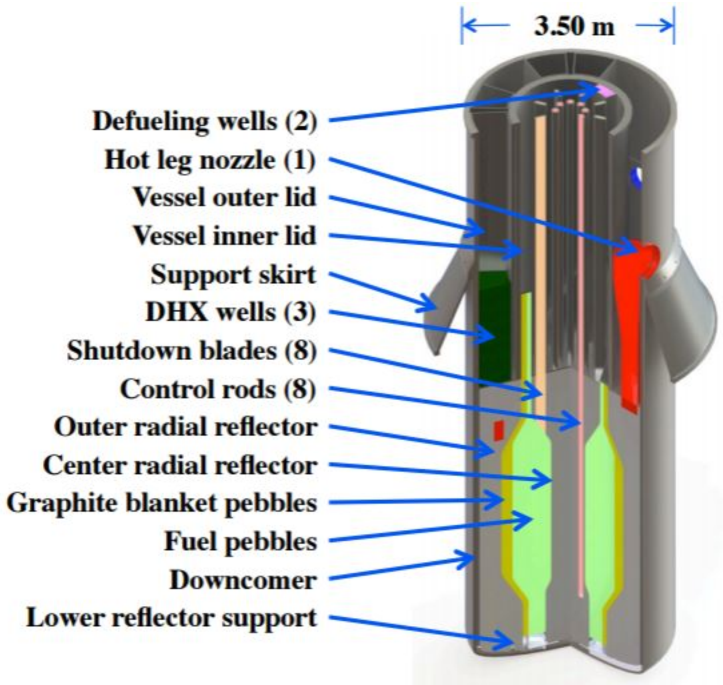

Figure 7 – PB-FHR Core

The pebbles, seen in Figure 8, are fueled with the same TRISO fuel particles as the AHTR. These pebbles consist of one high-density graphite outer surface layer, an annulus of TRISO fuel, and a low-density graphite core.

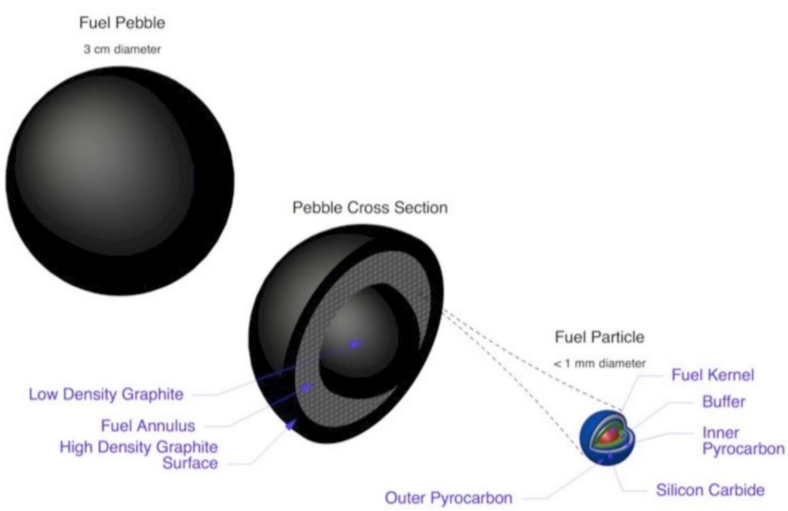

Figure 8 – Fuel Pebble

2. Codes Overview

This section contains a high-level overview of many codes, as well as information about their past and possible applicability to FHRs. The codes are broadly categorized into the same three groups as the M&S Workshop breakout sessions: neutronics, thermal-hydraulics, and materials.

2.1. Neutronics

2.1.1. SCALE

The SCALE Code System is a production level suite of tools that has been continuously deployed, enhanced, and supported since 1980 under sponsorship from the U.S. Nuclear Regulatory Commission and the U.S. Department of Energy. SCALE includes a number of computational modules integrated into sequences that address a wide variety of applications, including reactor physics, criticality safety, spent fuel characterization, source term analysis, radiation shielding, and sensitivity/uncertainty quantification. SCALE also includes continuous energy (CE) and multi-group (MG) cross section libraries in several group structures; best available nuclear data for depletion, decay and activation analysis; as well as the best available covariance libraries describing nuclear data uncertainties and correlations (Rearden, B. T.; Jessee, M. T.; Eds., 2016).

SCALE 6.2, the latest release, brings improved accuracy and significant reductions in both run-time and memory requirements for many sequences, as well as improved efficiency for parallel Monte Carlo computations. A new unified graphic user interface called Fulcrum is available for simplified and consistent user input to essentially all sequences. Fulcrum also coordinates user input with rendering of Monte Carlo models and plots output results and nuclear data (Rearden, et al., 2017).

Most sequences in SCALE 6.2 can be applied directly to FHR simulations, though enhancements and extensions may be necessary in some cases. Although CE data are applicable to all system types, MG nuclear data libraries tailored to FHR spectra and physics also should be processed. SCALE 6.2 provides many capabilities that will facilitate the analysis of FHRs.

1. SCALE 6.1 and earlier versions provide MG self-shielding of doubly-heterogeneous tristructural-isotropic (TRISO) fuel that are improved and extended in SCALE 6.2 to include plate fuel geometry in FHRs, in addition to spherical, cylindrical geometry for regular, asymmetric, and annular fuel elements.
2. SCALE 6.2 introduces problem-dependent Doppler broadening in CE Monte Carlo calculations for resolved and unresolved resonances as well as thermal scattering data to address spatial variations of temperature in FHR fuel as well as parallel calculation capabilities in KENO.
3. SCALE 6.2 provides MG and CE shielding analysis with hybrid deterministic-Monte Carlo calculations, which can reduce the Monte Carlo execution time by orders of magnitude.

4. The characterization of tritium production from lithium based salts has been substantially improved in SCALE 6.2 and compared with the limited validation data available from the Molten Salt Reactor Experiment (Briggs, Winter 1971-1972).
5. SCALE 6.2 introduces sensitivity/uncertainty analysis with the new Sampler tool as well as CE Monte Carlo analysis of eigenvalues as well as reaction rates with TSUNAMI-3D. SCALE's library of nuclear data uncertainties have also been significantly updated to include the latest data available from ENDF/B-VII.1. These tools can be applied to quantify uncertainties in FHR calculations as well as identify applicable neutronics benchmarks for validation.
6. Processing of MG and CE data for SCALE are performed with the AMPX code system, which is now distributed with SCALE 6.2. AMPX can be used to easily generate specialized libraries for FHR analysis, which will be important for determining optimized group structures.

2.1.2. MCNP

The Monte Carlo N-Particle (MCNP) transport code is developed and provided by the Radiation Safety Information Computation Center (RSICC). MCNP uses continuous energy cross-sections and because of its generalized geometry capability can model multitude of complicated core and reactor geometries. MCNP is a stochastic neutron, photon, and electron transport code that can perform both fixed sources and criticality (eigenvalue) calculations. As a result, the code has many applications in areas such as radiation protection and dosimetry, radiation shielding, reactor physics, and medical physics (MCNP, 2013). In particular, MCNP also has the capability to model the physics performance of instrumentation and sensors for reactors including FHRs.

MCNP limitations for FHR modeling and simulation are mainly two-fold: (1) fission source convergence in eigenvalue problems, and (2) computational efficiency, particularly when detailed (local) solutions (tally) is required, as is the case in realistic reactor analysis. A common problem with all codes is the lack of cross section data for certain materials used in FHR designs (e.g., scattering kernel for graphite and FLiBe).

2.1.3. NEAMS Toolkit

The mission of the US Department of Energy's Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program is to develop, apply, deploy, and support state-of-the-art predictive modeling and simulation tools for the design and analysis of current and future nuclear energy systems using computing architectures from laptops to leadership-class facilities. The tools in the NEAMS ToolKit will enable transformative scientific discovery and insights otherwise not attainable or affordable and will accelerate the solutions to existing problems as well as the deployment of new designs for current and advanced reactors. These tools will be applied to solve problems identified as significant by industry and consequently will expand validation, application, and long-term utility of these advanced tools.

The NEAMS program is organized along three product lines: the Fuels Product Line (FPL), the Reactors Product Line (RPL) and the Integration Product Line (IPL). The NEAMS FPL provides advanced tools for the analysis of current and future fuel types with the BISON and MARMOT tools based on the Multiphysics Object-Oriented Simulation Environment (MOOSE) from Idaho National Laboratory (INL). These tools have been validated for light water reactor fuels and demonstrated for the analysis of TRISO fuels. The NEAMS RPL includes the PROTEUS neutronics system (including neutron transport code, multi-group cross section generation codes, and spatial mesh generation tools), the SAM system analysis code, and the NEK5000 computational fluid dynamics code from SHARP tools from Argonne National Laboratory. The SHARP tools were initially developed for sodium-cooled fast reactor (SFR) technologies but could be applied for applications to advanced reactors such as FHRs. The NEAMS IPL, led at ORNL, is responding to the needs of design and analysis communities by integrating the advance NEAMS multiphysics capabilities and current production tools in an easy-to-use common analysis environment that enables end users to apply high-fidelity simulations to inform lower-order models for the design, analysis, and licensing of advanced nuclear systems, especially through the NEAMS Workbench (Rearden, Lefebvre, Thompson, Langley, & Stauff, April 16-20, 2017). Ongoing development of the Warthog multiphysics tool will provide the ability to use the PROTEUS neutron transport solver through a MOOSE application and include cross sections generated with SCALE for double-heterogeneity fuel, described in another section of this report, along with BISON fuel performance calculations (Hard, 2016).

The NEAMS ToolKit integrates various codes for advanced reactor analysis including the ability to prepare multi-group cross sectional data, perform neutronics calculations, generate depletion/source terms, run thermal hydraulics systems, analyze fuel performance, perform structural analysis, and calculate uncertainty quantities. Current challenges with the NEAMS toolset, particularly in neutronics, are as follows: (1) Modeling complicated geometries with multiple heterogeneities typical to the two FHR designs considered in this whitepaper. This issue may present itself in multi-group cross section generation (using MC^2-3, the cross section API, or Monte Carlo codes) and a potential need for homogenization due to excessive spatial meshing required to model the heterogeneities, (2) Computational efficiency associated with deterministic transport methods in modeling large reactor systems/cores, (3) Accessibility of the tools in the community and limited but growing user base.

2.1.4. ARGONNE REACTOR CODES

The Argonne Reactor Codes (ARC) system comprises a consistent compilation of MC^2-3, DIF3D, REBUS-3, VARI3D, PERSENT, and associated utilities. MC^2-3 is the multi-group cross section generation tool for DIF3D as well as PROTEUS. DIF3D is the diffusion and transport theory solver for neutrons and gammas. REBUS-3 is a generic fuel cycle analysis code built around DIF3D. PERSENT and VARI3D are perturbation and sensitivity analysis tools built around DIF3D. Based on homogeneous assemblies, the ARC system has been well verified and validated for fast reactor design and analysis and in addition were updated for prismatic-type Very High Temperature Reactor (VHTR) analysis (Argonne National Laboratory, 2014).

With additional updates, the ARC system could be applied to analyzing prismatic-type FHRs, but spatial homogenization and multi-group cross sections would be challenging issues in accurately modeling FHRs. The Workbench may allow users to easily access and combine useful features and capabilities from external tools such as SCALE.

2.1.5. COMET

COMET is an advanced continuous energy hybrid stochastic deterministic transport code with stochastic method fidelity such as that of MCNP but with computational speeds several orders of magnitude faster. COMET works by decomposing a large, heterogeneous system into a set of smaller fixed source local problems. For each unique local problem (e.g., fuel assembly types) that exists, a solution called the response function is obtained. These response functions are pre-computed as a library for future use by resolving the set of smaller fixed source problems. The overall solution to the global problem is then obtained by repeatedly generating local solutions via a linear superposition of responses for the unique local problems.

COMET's computational efficiency and ability to model complex geometries make it an ideal candidate for neutronics modeling of AHTR or other reactor core design with high heterogeneity. COMET has been shown to be highly accurate for current Light and Heavy Water Reactors (LWR and CANDU), the Very High Temperature Reactor (VHTR), the Hight Temperature Test Reactor (HTTR), and the Advanced Burner Test Reactor (ABTR) at steady state.

Two new modules/codes have been developed to advance the COMET framework – the Stochastic Particle Response Calculator (SPaRC) and the Application Programming Interface for Depletion Analysis (APIDA). These modules will extend COMET for lattice and core depletion calculations. Recently, further efficiency improvements have been made through adaptive flux expansion and parallel computing in COMET. The observed speedup on 40 processors for the parallel version is about 25 (depending on the reactor configuration) with an additional speedup factor of 2-4 times when the adaptive method/option is used.

Disclosure: The first author owns equity in a company that has licensed the COMET technologies from Georgia Tech. This description of COMET could affect his personal financial status. The terms of this arrangement have been reviewed and approved by Georgia Tech in accordance with its conflict of interest policies.

2.1.6. SERPENT

SERPENT is a three-dimensional continuous-energy Monte Carlo particle transport code. Its advantages and limitations are similar to MCNP. However, it is computationally more efficient because of the use of unionized energy grid and it is geared more for reactor physics calculation including depletion. Because SERPENT is a recently developed computational tool, the validation base for SERPENT is limited but growing worldwide

(Leppanen et al., 2015). SERPENT was originally developed for cross section generation and conducting depletion calculations, but has continued to mature to include multi-physics capabilities, higher- energy capabilities for fusion applications, and dose rates for medical physics. For any Monte Carlo code being applied specifically toward this project though, the most important question comes down to the ease of accurately treating the TRISO fuel particles. From a coding implementation standpoint, SERPENT can relatively easily model randomly dispersed TRISO particles. SERPENT has a separate command line routine which creates a separate random particle location geometry file, which is then read when executing a transport simulation.

However, like most other Monte Carlo codes, modeling the double heterogeneity of the TRISO fuel still presents computational challenges for SERPENT. In order to accurately capture the effect of having randomly dispersed particles, fuel kernel locations need to be explicitly declared through the input geometry. This can require a moderately higher amount of computational overhead depending on the model complexity and also increases the execution time versus a lattice calculation.

2.2. Thermal-Hydraulics

2.2.1. RELAP5, RELAP5/MOD3, RELAP5-3D

RELAP5 (Reactor Excursion and Leakage Analysis Program) is a system analysis code developed at INL for best-estimate transient simulation of light water reactor accident scenarios. It allows the modeling of the cooling system coupled to the core in the following typical accident conditions: loss of coolant accident (LOCA), anticipated transients with scram (ATWS), loss of offsite power (LOOP), loss of feedwater and loss of flow. A variety of thermal hydraulic systems can be simulated, including control system and secondary system components

The code was originally designed for LWRs, but its general framework is potentially applicable to advanced reactors, such as FHRs. RELAP5 is capable of modeling a wide variety of operational and accident conditions, for design and safety analysis purposes. However, RELAP5 does not feature heat transfer and friction correlations typically used for advanced reactor (plate fuel and pebble bed cores) (Sun, Yoder, & Christensen, 2016).

Extensive validation is needed to qualify RELAP5 for use for FHR simulations and identify needed further modifications and improvements to make sure the modeling approach is suitable for FHRs.

2.2.2. TRACE

TRACE (TRAC/RELAP Advanced Computational Engine) is the latest and most advanced best-estimate reactor system code developed by the US Nuclear Regulatory Commission for analyzing transient and steady-state neutronic and thermal-hydraulic behavior in LWRs. It is used to analyze operational transients, LOCA, and other accident scenarios in PWRs and BWRs. This code features modeling capabilities for multidimensional two-phase flow, non-equilibrium thermodynamics, generalized heat transfer, reflood, level tracking and reactor kinetics.

TRACE was designed for LWRs. Integration into the SNAP GUI and coupling with PARCS 3D nodal kinetics are available and easily accessible. The official TRACE release does not currently feature explicit modeling capabilities for salt-based systems. However, the code is generally applicable to non-water-based systems, and modified code versions exist which include thermophysical properties and correlations suitable for molten salts. Recently, TRACE has been used for preliminary modeling of the AHTR and experimental facilities at ORNL (Sun, Yoder, & Christensen, 2016).

2.2.3. SAM

The System Analysis Module (SAM) is an advanced and modern system analysis tool being developed under the U.S. DOE Office of Nuclear Energy's NEAMS program (Hu, 2017). SAM development aims for advances in physical modeling, numerical methods, and software engineering to enhance its user experience and usability. To facilitate the code development, SAM utilizes an object-oriented application framework (MOOSE), and its underlying meshing and finite-element library (libMesh) and linear and non-linear solvers (PETSc), to leverage the modern advanced software environments and numerical methods. It incorporates advances in the physical and empirical models as well as seeking the closure models derived based on information from high-fidelity simulations and experiments. Coupling interfaces have been developed to allow for convenient integration with other advanced or conventional simulation tools for multi-scale and multi-physics modeling capabilities.

SAM is being developed as a system-level modeling and simulation tool with higher fidelity but yet computationally efficient. The initial effort has been focused on the modeling and simulation capabilities of the heat transfer and single-phase fluid dynamics responses in the SFR systems. The transient simulation capabilities of typical reactor accidents have been demonstrated in the transient simulations of the Advanced Burner Test Reactor and validated against the EBR-II benchmark test results. Additionally, a three-dimensional module is under development to model the multi-dimensional flow and thermal stratification phenomena in large enclosures for safety analysis. An advanced and efficient 3D flow modeling capability embedded in a system analysis code is very desirable to improve the accuracy of reactor safety analyses and to reduce modeling uncertainties. It is anticipated that with limited modifications/additions to SAM, it would be applicable to other single-phase fluid systems. With growing interests in MSR and FHR development, SAM capabilities are also being enhanced to address some MSR/FHR specific modeling needs, including built-in salt properties, radiation heat transport, salt freezing, liquid fuel transport, etc.

2.2.4. ANSYS Fluent

ANSYS Fluent is a commercial CFD software tool that includes well-validated physical modeling capabilities to deliver fast and accurate results across different applications.

It has been used for simulation and design of several components of liquid-salt-cooled reactors, such as diodicity and primary heat exchangers. It presents the typical challenges of CFD codes, namely large computational requirements (particularly for transient simulations of large systems), need for verification and validation of the results, and integration with other multiphysics tools.

2.2.5. STAR-CCM+

STAR-CCM+ is a commercial computer-aided engineering package developed by CD-Adapco. Originally developed as a CFD simulation tool, it has been expanded to include continuum mechanics, heat transfer and solid stress models. It can be used to solve problems involving multiphysics and complex geometries. The code can be coupled to neutronics codes, both deterministic and Mote Carlo. There is an extensive history of use with MCNP and most recently with SERPENT.

STAR-CCM+ has been used at ORNL to simulate the flow and thermal characteristics of the AHTR fuel assembly. It is currently being used at several national laboratories and universities for CFD and heat transfer applications (Sun, Yoder, & Christensen, 2016).

2.2.6. COMSOL

COMSOL Multiphysics is a finite element analysis solver and simulation software package for various physics and engineering applications, especially coupled and multiphysics phenomena. The package features an application builder and a physics builder that allow for creating specialized and customized models that integrate with the standard models. COMSOL has been used for CFD analysis of heat transfer for FHR-DR assembly, simulation of the flow distribution for the Pebble-bed AHTR, and other multiphysics applications involving liquid salts.

2.2.7. OpenFOAM

OpenFOAM (Open source Field Operation And Manipulation) is a C++ toolbox for the development of customized numerical solvers for solution of continuum mechanics problems, including CFD. The code is open source, thus allowing anyone to have access to this code.

The code has been used for flow simulation of molten salt reactors, as well as pebble-bed liquid-salt reactors, coupled with the neutronics Monte Carlo code SERPENT.

2.2.8. NEK5000

Nek5000 is an open-source, highly scalable and portable spectral element code designed to simulate unsteady Stokes, unsteady incompressible Navier-Stokes, low Mach-number flows, heat transfer and species transport and incompressible magnetohydrodynamics (MHD). It is part of the NEAMS program and provides the following features:

- Scalability to over a million processors;

- High-order spatial and temporal discretization
- Highly optimized computational performance
- Capability for solution of incompressible + low Mach number (variable density) flows

2.3. Materials

2.3.1. MOOSE

The Multiphysics Object-Oriented Simulation Environment (MOOSE) is a finite-element, fully coupled, fully implicit, multiphysics framework. MOOSE has modules for solid mechanics, Navier-Stokes, heat conduction, phase field modeling, and more. Some other capabilities included dimension independent physics, built-in mesh adaptively, and continuous and discontinuous Galerkin.

2.3.2. BISON

BISON is a finite element nuclear fuel performance code developed from MOOSE. BISON is applicable to a variety of fuel forms including TRISO particle fuel and plate fuel. BISON solves the fully-coupled equations of thermomechanics and species diffusion, from 1D spherical to 3D geometries. Models included can describe densification, swelling, temperature and burnup dependent thermal properties, fracture, thermal and irradiation creep, and fission gas production and release. BISON has been coupled with MARMOT, a mesoscale fuel performance that is also based on MOOSE.

2.3.3. MARMOT

The purpose of MARMOT is to predict the coevolution of microstructure and material properties of nuclear fuels and claddings due to stress, temperature, and irradiation damage. It then supplies microstructural material models to BISON. MARMOT solves the phase field equations coupled to solid mechanics and heat conduction using the finite element method.

2.3.4. Structural Material Codes

Codes for modeling the chemical degradation (corrosion) of structural materials have not been applied to FHR environments. However, 3D corrosion modeling has been done in a comparable salt environment, for molten chloride salt coolant in high- temperature concentrated solar power (CSP) generation. One important corrosion mechanism common to both FHRs and molten chloride CSP is temperature gradient driven mass transfer, whereby chromium from structural materials in hot areas of a flow loop dissolves and is transported to the surfaces of materials in cooler areas. Tavakoli et al. demonstrated a 3D model using the commercial CFD code STAR-CD which coupled CFD to electrochemical kinetics of corrosion reactions with mass and heat transfer (Tavakoli 2016). These models have predicted corrosion rates and corrosion potentials which agree with experimental results for nickel alloys. These methods could be applied to FHR systems.

Radiation damage of structural materials can be modeled using four main classes of tools. These include atomistic methods ab initio calculations, molecular dynamics, and lattice Monte Carlo, as well as rate theory and object Monte Carlo for mesoscopic/continuum scale (Stoller 2005). However, modeling of this type is meant to understand how radiation affects in materials properties of irradiated materials, and cannot be used to directly predict how radiation affects the functionality of specific structural components as they are arranged in a reactor system. Additionally, the synergistic effect radiation has with chemical corrosion is not captured by these methods.

Overall, there are currently very few codes that model the degradation of structural materials in a fluoride high-temperature reactor. Due to the fact that codes focus on an idealized model of materials, it is difficult to accept the results of code-based material analysis. More work needs to be done to investigate degradation effects before a code can be created for such a purpose.

3. Initial Broad FHR Modeling & Simulation Challenges

As a starting point to determine the phenomena that potentially need to be addressed in support of licensing of the FHR M&S tools, the Georgia Tech led IRP convened Phenomena Identification and Ranking Table (PIRT) panels of both internal and external experts. The results of the PIRT panel meetings for neutronics, thermal hydraulics, materials, and multiphysics are provided in PIRT reports. All the PIRT reports have been published except the Multiphysics Report. The PIRT phenomena relevant to modeling and simulation are summarized below. These results represent the broader, global issues related to M&S of FHRs specifically, and are expected to facilitate more accurate modeling as they are addressed.

Listed below are the phenomena identified by each PIRT panel as being of high or medium relative importance, with a relatively low level of knowledge of the subject. In the full PIRT reports, each phenomenon matching those characteristics was given a path forward to begin to bridge the gap. These paths forward are omitted here due to length.

Additionally, information about M&S of FHR instrumentation is provided. Although not the result of a PIRT meeting, it is included in this section to provide background on the subject for consideration in the development of FHR M&S tools.

3.1. PIRT – Neutronics

The PIRTs related to neutronics were broken into four categories: fundamental cross section data, material composition, computational modeling, and spectral history effects. Of these, issues relating to both fundamental cross section data and material composition are universal to all codes. Computational methodology and general depletion issues can vary from code set to code set. (Rahnema, Edgar, Zhang, & Petrovic, 2016)

3.1.1. Fundamental Cross Section Data

There are five phenomena related to fundamental cross section data:

- Moderation in FLiBe
- Thermalization in FLiBe
- Absorption in FLiBe
- Thermalization in carbon
- Absorption in carbon

The PIRT report describes the specific pathway for each of these phenomena, but the net result associated with addressing these phenomena is a cross section library containing improvements in areas of specific interest to FHRs. As mentioned above, these five issues are universal to all code sets, as they all are inherently limited by the quality of the underlying cross section data.

3.1.2. Material Composition

The only issue identified under the category of material composition is that of the fuel particle distribution. Relevant to both the AHTR and Mk1 PB-FHR designs, the distribution of TRISO particles in real fabricated fuel is not well known. This could have implications in key reactor parameters like k_{eff} and peaking factors.

Obtaining data on this distribution is relevant to all codes, as this affects the geometry of the underlying model. However, the ability of the code to accurately and quickly model this distribution can vary, and should be considered.

3.1.3. Computational Methodology

At ten identified phenomena, computational methodology is the largest area of improvement:

- Solution convergence
- Granularity of depletion regions
- Multiple heterogeneity treatment for generating multi-group cross sections
- Selection of multi-group structure
- Boundary conditions for multi-group cross section generation
- Burnable poison cell
- Scattering kernel
- Spatial mesh
- Diffusion approximation
- Dehomogenization if relevant

These phenomena can be roughly grouped into issues of solution convergence, multi-group treatment, and solution method approximations. Addressing these phenomena would result in a base of knowledge about how to use existing codes to accurately model FHRs, or an adapted version of an existing code that is optimized for FHRs.

3.1.4. General Depletion

The only identified issue related to general depletion is that of spectral history effects. While well understood in LWRs, these methods have yet to be adapted to FHRs. Sensitivity analyses relating to the effect of the spectral history of the reactor must be performed, and these methods must be adapted to FHR modeling codes.

3.2. PIRT – Thermal-Hydraulics

The thermal-hydraulics PIRT exercise first identified a list of accident scenarios that are considered to be of paramount importance in eventual licensing, with AHTR as a reference FHR design. Due to time constraints, two scenarios were selected for focus with detailed discussion: station blackout and simultaneous withdrawal of control rods. Within these two accident scenarios, phenomena were identified and ranked in terms of importance as well as the knowledge base associated with these phenomena (Sun X. , et al., 2016).

3.2.1. Station Blackout

Within the station blackout scenario, the following thirteen phenomena were identified as needing further study in order to understand and accurately model the accident:

- Geometry of the fuel plate (deviation from nominal geometry)
- Thermal conductivity of FLiBe
- Viscosity of FLiBe
- Wall friction in the core
- Core flow asymmetry
- Upper plenum mixing
- Lower plenum mixing
- Fluidic diodicity
- DHX performance
- NDHX performance
- DRACS piping heat loss
- Chimney natural circulation and performance
- KF-ZrF_4 thermo-physical properties

These specific phenomena culminate in the larger need for multi-dimensional detailed CFD models of the reactor vessel, including the downcomer region, lower plenum, core, upper plenum, DRACS heat exchangers, and modeling the accident scenario within this large-scale model.

3.2.2. Simultaneous Withdrawal of All Control Rods

The withdrawal of all control rods in the AHTR is unique due to its passive safety feature of fusible links between the control blades and the drive mechanism. These links are designed to melt at high temperatures, to allow the control blades to drop into the core.

To model this scenario, twelve phenomena were identified as needing further study:

- Thermal conductivity of FLiBe
- Viscosity of FLiBe
- Core heat transfer coefficient
- Core flow asymmetry
- Primary coolant flow bypass faction
- Upper plenum mixing
- Heat transfer to fusible links
- Primary pump performance
- P-IHX performance
- Intermediate pump performance
- I-PHX performance
- Power cycle performance

These phenomena culminate in the need of a multi-dimensional CFD model of the reactor core, as well as a system-level thermal-hydraulics model in order to simulate heat transfer at every stage, including the intermediate and power cycle loops.

3.3. PIRT – Materials

The materials pillar FHR-IRP project focuses on structural reactor materials, and the degradation mechanisms associated with reactor operation in a molten salt environment. The report (Singh, Chan, & Rahnema, 2017) is very detailed, and goes into knowledge levels of specific phenomena with regard to salt interaction with each proposed structural material. As such, its contents are not easy to summarize. However, as discussed above, no code set really exists that holistically models material degradation in this environment. Thus, it is apparent that the path forward in terms of material modeling involves aggregating these degradation mechanisms into one M&S kit.

The report examines many different materials in the context of different structural uses. Note, since the TRISO fuel particles used in these reactors are common to other high-temperature reactors such as the HTGR and VHTR, materials phenomena in the context of fuel is not discussed here. The report identified six structural applications:

- Vessel and Primary Piping
- Primary Heat Exchanger
- Steam Generator Tubes and Vessel
- Intermediate Loop Piping

- Valves and Pumps
- Welds

Within each material/use combination, different phenomena are identified. These phenomena include, but are not limited to,

- Cladding Interdiffusion
- Cladding Delamination
- Creep
- Fatigue
- Creep-Fatigue
- Crack Growth
- Stress Relaxation Cracking
- Irradiation Embrittlement

These phenomena are ranked in terms of knowledge and relative importance for each unique material/use combination.

3.4. PIRT – Multiphysics

A fourth PIRT panel was established for this project to examine the challenge of modeling coupled multiple simultaneous physical phenomena in FHRs. This area, called "multiphysics modeling", is desirable because it has the potential to significantly improve model fidelity and more accurately predict responses during reactor transients. The PIRT panel focused on three main operation scenarios: Normal Operation, Station Blackout, and Simultaneous Withdrawal of All Control Rods, as well as another category for phenomena that didn't fit one of these categories. Phenomena were defined as either requiring "Tight" or "Loose" coupling. Tight coupling is defined as requiring detailed iterative feedback between two codes/models. Loose coupling is defined as requiring the sharing of precalculated information between two codes. Phenomena identified as requiring "tight" coupling are examined below (Zhang, Rahnema, Avigni, & Petrovic, 2017).

3.4.1. Normal Operation

For the normal operation scenario, there were five phenomena identified as requiring "tight" coupling to accurately model:

- Energy generation rate in fuel kernel
- Assembly (graphite) reactivity feedback
- Coolant reactivity feedback
- Upper plenum mixing
- Heat transfer to fusible links

These five phenomena involve “tight” coupling between neutronics and thermal-hydraulics codes. The relative value of the accuracy gained from this “tight” coupling needs to be investigated.

3.4.2. Station Blackout

All phenomena identified in the station blackout scenario only require “loose” coupling. As such, they are not listed here.

3.4.3. Simultaneous Withdrawal of All Control Rods

Within the simultaneous withdrawal of all control rods scenario, five phenomena were identified as requiring “tight” coupling:

- Energy generation rate in kernel
- Fuel Temperature reactivity coefficient
- Assembly (graphite) reactivity coefficient
- Upper plenum mixing
- Heat transfer to fusible links

Much like the phenomena identified in the normal operation scenario, these phenomena require “tight” coupling of neutronics and thermal-hydraulics codes.

3.4.4. Other

Six “other” phenomena were identified as requiring “tight” coupling:

- Tube rupture in P-IHX
- Overcooling due to inadvertent DRACS operation or restart/shut down of primary pumps
- Secondary shut down system/kinetics and fluid mixing and dissolution in lower plenum
- Salt deposition on control rod drive mechanism
- Grid disconnection event
- Partial flow blockage accident

3.5. Instrumentation

The high-temperature, molten fluoride-salt coolant provides a harsh environment for nuclear reactor state and diagnostic sensors. Reactor instrumentation provides information for plant operation, automated control, and corrective action in abnormal situations. Reactor systems necessitate multiple systems measuring extensive parameters (temperature, pressure, neutron flux, etc.) to guard against single point failures and inadvertent reactor shutdown (International Atomic Energy Agency, 1999) . The instrumentation needs for first-of-a-kind research reactors are different than later generations of the research reactors as well as power generation reactors.

The same instrumentation technologies that are developed for the molten salt reactor will find application in any industry that utilizes molten salt heat transfer loops. These include, but are not limited to renewable energy power generation and storage, petrochemical production, and materials manufacturing.

Much, if not all, of commercially available nuclear reactor instrumentation is devoted to water cooled reactor technology. Instrumentation will need to be able to measure temperature, pressure, mass flow rate, flow velocity, two phase void fraction, and liquid levels under high-temperature (>500ºC), high-radiation, and corrosive environmental factors.

Fiber optic sensors have the potential for low-profile, robust instrumentation in the harsh environments of high-temperature, molten salt loops. They are immune from electromagnetic interference (EMI) at the location of measurement, and many sensors can be combined into a single fiber bundle to provide redundancy, greater awareness, or both. Fiber optic sensors have two broad classifications: extrinsic/hybrid or intrinsic/all-fiber. Extrinsic fiber sensors are similar to the conventional counterparts except that the measure of deflection is performed by light. Intrinsic fiber sensors use a change in the fiber itself as the measurement (Hashemian, 2011).

Simulation capabilities for instrumentation and sensor development and performance modeling do exist and involve the uses of codes like MCNP and CFD tools. However, use of these codes requires further increase in modeling details in the FHR models accounting for not only the reactor features but sensor physics. These will result in increased computational times. Availability of related modeling capabilities in deterministic tools would be desirable. Some of the physics models in MCNP are limited to empirical models and require generalizations for broader use for sensor simulations in larger models. As an example, ability to model Cerenkov emission spectra can be noted. The capability in MCNP does exist but requires further development.

The sections provided in Appendix A provide discussions on relevant instrumentation and sensor needs and related challenges for FHRs focusing flux, temperature, pressure and flow measurements. Depletion calculations provide capabilities to simulate sensor performance targeting composition evaluations as well.

4. FHR Modeling and Simulation Workshop Overview

On March 8-9, 2017, the Georgia Tech-led FHR-IRP team hosted a Modeling and Simulation Workshop. Close to 60 experts in the field were invited from universities, national laboratories, industry, the United States Nuclear Regulatory Commission, the United States Department of Energy, and Canadian Nuclear Laboratories. The purpose of this meeting was to:

- provide an opportunity for code developers to discuss the applicability of their code sets to the unique challenges posed by FHR modeling,
- allow researchers to discuss the ways in which they use various codes in their FHR research,
- create a forum where researchers and developers can collaborate and discuss gaps and needs of codes with respect to FHR modeling.

The first day of the workshop included presentations from a diverse group of presenters, including executives from DOE, DOE national labs, industry, and others. These presentations discussed capabilities of contemporary code sets with respect to FHR modeling, as well as current goals for FHR research and development.

The second day of the workshop consisted of three breakout sessions – one each for thermal-hydraulics, neutronics, and materials – where modeling issues more specifically related to each field were discussed and categorized. The results of these breakout sessions are discussed in Section 5 of this document.

4.1.1. Agenda

Workshop on Tools for Modeling and Simulation of Fluoride Cooled High Temperature Reactors (FHR)
Organized Jointly by Georgia Institute of Technology, MIT, and UCB
3/8-9/2017
GTMI Auditorium
Georgia Institute of Technology
813 Ferst Dr NW, Atlanta, GA 30332
Georgia Institute of Technology

Objective: The objective of the workshop is to review the capabilities of the current modeling and simulation (M&S) tools for multi physics analysis of the FHRs and to identify the gaps and needs for the development, extension, and/or V&V of existing tools necessary to support the licensing of the FHRs. A whitepaper will be drafted for this workshop and will be finalized based on the workshop results. The document can potentially serve as an initiative by DOE-NE.

AGENDA (March 8, 2017)

07:00am Continental breakfast and registration

Keynote Speakers

08:00 Welcome and introduction

08:20 Importance of modeling and simulation tools for advanced reactors – Dan Funk for Shane Johnson (DOE-NE)

Moderator – Dan Funk (DOE-NE)

08:30 Remarks by the National Technical Director for Molten Salt Reactors – Lou Qualls (ORNL)

08:35 GAIN initiative updates – Rita Baranwal (GAIN)

08:45 EPRI / GAIN Modeling and Simulation (M&S) Initiative – Cristian Marciulescu (EPRI)

08:50 Kairos Power – Ed Blandford (Kairos Power)

09:10 FHR Licensing – George Flanagan (ORNL)

M&S capabilities for AHTR & PB-FHR analysis

09:30 FHR & MSR modeling tools: past, present, and future – Lou Qualls (ORNL)

10:00 Break

Moderators – Paul Burke, Kyle Ramey

10:25 SCALE Enhancements for Advanced Reactor Analysis– Brad Rearden (ORNL)

10:55 An Introduction to NEAMS Workbench – Brad Rearden (ORNL)

11:25 A Multiscale FHR Modeling and Simulation Approach Employing NEAMS Tools – Rich Martineau (INL)

12:00 Lunch

01:30pm NEAMS/SHARP tool set – Elia Merzari (ANL)

02:00 SAM tool set – Rui Hu (ANL)

02:30 TRACE/PARCS tool set - Aaron Wysocki (ORNL)

03:00 Modelling of Advanced Reactor Concepts at CNL– Alex Levinsky (CNL)

03:30 Break

Moderators – Hemin Noorani, Giovanni Maronati

04:00 COMET tool set – Farzad Rahnema (GIT)

04:30 Current tools in use by Georgia Tech for AHTR analysis – Bojan Petrovic (GIT)

05:00 Current tools in use by UCB for PB-FHR analysis – Max Fratoni (UCB)

05:30 Issues with modeling and simulation of tritium management in salt system – Pattrick Calderoni (INL)

06:00 Adjourn

06:00-08:00pm Reception

AGENDA (March 9, 2017) – Breakout sessions, discussion, and wrap up

07:30am Continental breakfast

08:30 Instructions and format for the breakout session – Farzad Rahnema

Objective: To identify gaps and needs for the development and/or extension of tools and V&V

08:45 Breakout sessions
- Neutronics – GTMI, auditorium
  Leads: Bojan Petrovic, Farzad Rahnema, Max Fratoni, and Paul Burke
- Thermal fluids/hydraulics – Boggs, 3-28
  Leads: Xiaodong Sun, Grady Yoder, and Carl Stoots, and Pietro Avigni
- Materials – Boggs, 3-39
  Leads: Preet Singh and Jinsuo Zhang, Kevin Chan

10:00 Break

10:30 Breakout sessions continue

11:30 Lunch – CASL tool set – Ben Collins for Jess Gehin (ORNL)

1:00 Summary of neutronics breakout session – Farzad Rahnema/Bojan Petrovic/ Max Fratoni

1:40 Summary of thermal hydraulics breakout session – Xiaodong Sun/Grady Yoder/Carl Stoots

2:20 Break

2:50 Summary of materials breakout session – Preet Singh/Jinsuo Zhang

3:30 Wrap up and path forward – Farzad Rahnema

4:00 Adjourn

4.1.2. Attendee List

Aaron Wysocki	James Kendrick
Abdalla Jaoude	Jian Ruan
Akshay Dave	Jinsuo Zhang
Alexandra Zuchkova	Joseph Farleo
Anil Prinja	Kaichao Sun
April Novak	Karl Birsch
Bojan Petrovic	Kumar Sridhran
Brad Rearden	Lou Qualls
Brandon Haugh	Max Fratoni
Carl Stoots	Michael Huang
Chaitanya Deo	Nick Smith
Chris Poresky	Nisarg Patel
Cristian Marciulescu	Pattrick Calderoni
Dan Funk	Paul Burke

Dan Ilas	Pietro Avigni
Dingkang Zhang	Preet Singh
Ed Blandford	Raluca Scarlat
Elia Merzari	Richard Martineau
Farzad rahnema	Rita Baranwal
Florent Heidet	Rui Hu
George Flanagan - Remote	Stefano Terlizzi
Giovanni Maronati	Thomas Winter
Grady Yoder	Tim Flaspoehler
Harry Andreades	Wei Shen
Hemin Noorani	Xiaodong Sun
Hsun-Chia Lin	

4.1.3. Group Photo

5. Workshop Summary/Results

This section contains summaries of the results of the discussion in the three breakout sessions at the FHR M&S Workshop. Breakout session moderators began with an overview of modeling challenges previously identified during a one day meeting between the two FHR-IRP teams, based on the respective PIRT exercise performed by the Georgia Tech-led IRP. Breakout session attendees were then guided to discuss the relative capabilities of current codes, gaps that need to be addressed, and areas for future development.

5.1.1. Neutronics

The workshop results presented in this section highlight potential issues with the capabilities of current codes for modeling FHRs as per the workshop objective, whereas the PIRT panel results (Section 3.1) cover a broader set of issues which must be kept in perspective. For example, issues with fundamental cross section data are common to all neutronic codes. As such, these issues are not discussed here, but can be found in Section 3.1.1.

The first result of the neutronics breakout session was the conclusion that computation time can be prohibitively large for accurate modeling of FHRs. With regard to stochastic codes, the computation time associated with modeling large cores in full detail can be too large to be reasonable. Although certain stochastic codes may be more efficient using certain approximations (e.g., delta tracking in SERPENT), efficiency is still an issue. With regard to deterministic transport codes, computation time is a bigger issue for similar accuracy because of refined phase space discretization.

Next, two individual code sets were discussed, beginning with neutronics modeling in SCALE. SCALE includes a sequence for Monte Carlo neutron transport in multi-group and continuous energy modes. The use of deterministic transport for multi-group cross section generation for systems that contain multiple heterogeneity must be studied. Additionally, the impact of spectral effects on multi-group cross section generation must be studied.

The use and integration of the NEAMS toolkit was also discussed. It was assessed that the deterministic transport capabilities provided by the NEAMS toolkit are not adequately suited for modeling the PB-FHR or the AHTR, with efficiency and cross section generation being significant issues. Additionally, it was determined that for NEAMS to be a truly comprehensive kit, it must include a stochastic code for reference solution generation. For integration with other codes, it was reiterated that the planned generalized interface for mesh-based code integration would be very useful.

Finally, for FHR neutronics modeling, a list of issues and recommendations was developed.

- Small boron concentration in graphite can have a large effect on reactivity. However, boron (or boron equivalent) concentration in graphite is regulated by standards. For nuclear grade graphite, the concentration is limited to 2ppm. This is taken into account at the design stage. However, it is believed that other industries have clean graphite that can make this a non-issue.

- Cross section issues for in-core graphite and salt can result due to materials introduced during reactor operation. For example, material transferred to salt due to corrosion of structural material can become trapped in graphite. Another example is the materials added to the salt for redox control.
- For neutronics codes to be most useful in material integrity/lifetime calculations, it is recommended to identify the relevant physical parameters (e.g., DPA or fast fluence).
- Core transient calculation capabilities are an issue for FHRs.
    - SCALE does not have time-dependent calculation capability.
    - NEAMS capabilities in this regard are limited due to its use of the adiabatic model.
    - The system code RELAP5 by itself is not sufficient for this purpose, but can be used to model prismatic core transients when coupled to the reactor physics code PHISICS (not part of NEAMS or MOOSE). However, the feasibility of this approach for FHRs must be tested because of the difference in coolants (gas vs. salt). A similar approach, coupling RELAP7 to Rattlesnake (a 3D transport module from NEAMS), needs to be tested for FHRs.
- Multi-group cross-section generation to account for multiple heterogeneity in FHRs is non-trivial and computationally intensive. For the AHTR, the iterative Dancoff, RPT (Reactivity-equivalent Physical Transformation), and Sanchez/Pomraning methods have been used with limited success. There could be a potential issue with the thin fuel layers as is the case in the AHTR fuel plates (where fuel particles are embedded near the edges of the plates). These corrections when generated at beginning-of-cycle conditions can be used for depleted fuel with some small error. For the PB-FHR, current practice is to perform whole-core SERPENT calculations at different points in the core lifetime to generate multi-group cross sections for diffusion theory core calculations. While this method yields reasonable results, the redundancy of the whole-core Monte Carlo calculations makes it impractical for production calculations.
- Determining an efficient multi-group structure for FHR core calculations is not trivial, and needs to be studied. An optimization method to determine both coarse and fine group structures was recommended.
- Additional modeling issues specific to PB-FHR are listed below.
    - Coupling Monte Carlo codes to the mesh-based CFD code NEK5000 is not mature. The coupling of the Monte Carlo codes OpenMC and SHIFT to NEK5000 is under development. Currently, the PB-FHR is modeled using the Monte Carlo code SERPENT coupled with the CFD code OpenFOAM. This approach is mature, because the delta tracking method in SERPENT makes coupling to the volume-based OpenFOAM seamless.
    - Effects of pebble packing pattern and packing factor are significant in core calculations and calculating control rod worth. Modeling packing variation in the core by diffusion theory is difficult because of the homogenization (larger error at outer edge).
    - Diffusion theory calculations have issues with control rod modeling.

- However, it was noted that control rod depletion modeling may not be an issue (not needed) because of low excess reactivity due to pebble recirculation.

5.1.2. Thermal-Hydraulics

The workshop results presented in this section highlight potential issues with the capabilities of current codes for modeling FHRs as per the workshop objective, whereas the PIRT panel results (Section 3.1) cover a broader set of phenomena which must be kept in perspective.

In considering the state of T/H M&S for FHRs, the breakout session attendees began by defining the context of discussion via an example list of possible scenarios and initiating events, and a list of code sets and methodologies considered. In this context, the session produced a categorized set of modeling challenges, gaps in data, and phenomena that need further investigation.

The example scenarios and initiating events considered for the breakout session are:

- Station blackout (SBO)
- Simultaneous withdrawal of all control rods (SWCR)
- Prompt criticality
- Loss of forced circulation (LOFC)
- Partial flow blockage
- Loss of multiple DRACS loops
- Primary loop break, intermediate loop break, and vessel break

The code sets and methodologies considered in the breakout session are:

- System Level
    - RELAP5, TRACE
    - MoDSIM (Modelica based), SAM
    - Flownex
    - COBRA-TF (subchannel)
    - AGREE-PARCS, MELCOR, GRSAC
    - SFR codes for non-core issues (intermediate loops)
- CFD
    - ANSYS Fluent, STAR-CCM+, OpenFoam
    - NEK5000
    - COMSOL
- Coupled System-level and CFD Analysis
    - Flownex + Fluent
    - NEAMS Workbench, SAM-STAR-CCM+, SAM-NEK5000, …
    - COMSOL
- Multiphysics
    - Neutronics with T-H (reactivity feedback): Reactivity transients, core and subchannel response

- Materials, structural mechanics (thermal stress/creep/fluid-structure interactions), corrosion and precipitation, tritium transport, and T-H
- Porous Medium Approach
  - Pebble bed core
  - Plate fuel core
  - Prismatic core
- Multiscale Analysis
  - System/core/assembly/subchannels
  - Coupled system and CFD analysis

In this discussion context, a few broad challenges with FHR T/H M&S were identified. First, as with the neutronics breakout session, it was emphasized that large-scale simulations can be prohibitively expensive due to computation time. The use of parallel computing methods for these large-scale simulations can help to lower this barrier. Second, examining the list of initiating events, it became apparent that accurate modeling would require a multiphysics tool/method that included capabilities for effects such as salt freezing, corrosion, and precipitation. These effects require coupled multiphysics tools, which are not currently developed to a mature level. One of the challenges associated with the experiments, where electric heating is used to replace nuclear heating, is to determine the (simulated) transient reactor power using neutronics models. It was also discussed that current tools cannot simulate the entire reactor system response at a level that includes the power conversion system, which could have a significant effect on dynamic system response, when incorporated. Additionally, current multiphysics system dynamic response modeling capabilities do not include frequency response capabilities. Frequency response analysis has proved a very useful tool in analyzing system transients. The last broad challenge is that, for FHR, uncertainty analysis in these T/H experiments, including salt thermo-physical properties, and code calculations needs to be better understood, in order to be correctly propagated into grander statements about model accuracy.

The next result of the T/H breakout session is a list of gaps in current data libraries that need closing, such that the uncertainties due to inaccurate physical property data are reduced. The important physical properties are:

- Thermo-physical properties of salts (FLiBe, KF-ZrF_4, etc.)
  - Thermal conductivity
  - Viscosity
  - IR absorption (prototypic to salt conditions: temperature, purity level, composition, etc.)
  - Thermal expansion
  - Specific heat
  - Melting point at slightly off equilibrium salt eutectic composition (off stoichiometry) and with impurities
  - Properties at temperature ranging from operating temperatures to freezing point
  - Thermo-physical properties of salts with impurities (e.g., due to corrosion)

- Thermal conductivity and heat capacity of fresh and irradiated carbonaceous and structural materials over a broad temperature range
- Core heat transfer coefficient and wall friction factor for pebble bed, plate, and prismatic fuels

In addition, there are gaps in current codes pertaining to phenomena unique to FHRs. These areas for investigation are:

- Effect of salt thermal radiation as a participating medium for normal operation and accident conditions
- Flow oscillations in the core and upper plenum
- Lower plenum and upper plenum mixing, thermal stratification
- Heat transfer to upper plenum structural materials
- Thermal stress/fatigue/creep/cycling
- Fluid structure interactions
- Flow channel distortion/deformation due to swelling and thermal expansion (non-uniform neutron flux and temperature distribution, etc.)
- Primary coolant flow bypass fraction
- Core and downcomer flow asymmetry
- Heat exchanger steady-state and transient performance (P-IHX, I-PHX, DHX, and NDHX): including selection of the types of heat exchangers
- DRACS performance, fluidic diodicity (flow reversal), natural circulation
- Primary and intermediate loop pump performance
- Refueling and operational transients
- Extended fission product release for TRISO fuel
- Fission product transport and deposition
- Graphite oxidation
- Graphite dust (may not be as significant as for HTGR)

A summarizing conclusion from the above set of gaps is that there is a strong need for experimental data, including integral-effect, separate-effect, and mixed-effect tests. There is a relative lack of data with appropriate uncertainty quantification, and the above gaps cannot be closed without these experiments. The breakout session attendees were encouraged by test facilities (e.g., salt flow loops) available and being built around the world.

5.1.3. Materials

The workshop results presented in this section highlight potential issues with the capabilities of current codes for modeling FHRs as per the workshop objective, whereas the PIRT panel results (Section 3.1) cover a broader set of phenomena which must be kept in perspective.

Discussion on materials M&S led to conclusion that there was very little M&S activity for corrosion or degradation of structural materials in molten salts. Existing codes MOOSE and BISON are used mostly in fuel simulations. As a result, their applicability to structural material calculations is limited. Thermodynamic models are available (Thermocalc, Calphad, HSC, and others) which may be adapted for corrosion predictions. It was also concluded that there are gaps in the thermodynamic database needed for modeling corrosion, so a common-effort is needed to establish and validate the needed thermodynamic database for FHR material/environment system.

The possibility of coupling lower level physics codes (i.e. molecular dynamics) to upper level effects codes was discussed. Additionally, coupling materials and CFD codes was identified as an area of interest. This is due to the possible difference in chemistry resulting from the differences between flowing and stagnant zones. Therefore, there is a need to include mass transport models into thermal-hydraulics and corrosion models. Specifically, there is a need for steady state models to identify stagnant areas in a reactor. Corrosion modules could then be added to the thermohydraulic code, which may be in the form of thermodynamic calculations or an electrochemical corrosion model. An erosion-corrosion model may also be important for structural materials used in areas of high flow, as well as for the fuel particles.

It was also identified that real life situations and models could differ greatly due to a large amount of carbon (or other impurity) contamination with time, an effect which can be difficult to predict and thus model. There is a need to understand the source of carbon in salts, and mechanics such as its mass transport, possible reactions with metallic structure under operating conditions, etc.

One of the main conclusions of the materials breakout session was that there is a need for standardized ways to measure redox of FHR molten salts so that the results from different studies and under different conditions could be compared. Impurities in molten salts are the main reason for corrosion of structural materials in FHR environments, so it is essential that we have reliable standardized methods to quantify and control impurity levels in molten salt environments. Need of analytical methods to chemically analyze molten salts was highlighted. It was agreed that the there is a need to develop methods or sensors that will not only be useful for experimental studies but also in a working molten salt reactor to monitor and control salt chemistry. New spectroscopic methods to chemically analyze molten salts may be developed which take advantage of the optical properties of molten salts.

One other important concern was the lack of data on the effect of radiation on selected construction materials, newly developed or established alloys, and the synergistic effect of radiation and corrosion in FHR environments. There is a need for models to predict transmutation products and their effect on corrosivity of molten salts. Therefore, there is a need for corrosion/materials teams to coordinate with neutronics teams and establish a mutual feedback system. One specific concern in this area is the effect of tritium production in FHR and its effect of the salt chemistry and corrosion. Therefore, there is a need to develop models for tritium in FHR. It was agreed that there is a need to find alternatives to costly in-core loop experiments. This may be in terms of near-core loops or with simulated radiolysis chemistry loops.

Structural materials, especially metallic alloys, selected for FHRs must be code-approved to be used for reactor construction; therefore, it is essential to work towards code-readiness for licensing. There is a need for corrosion data for joints, welds, laminated structures, coatings, and thin components like heat exchangers. It is very important to generate essential long-term corrosion, mechanical behavior and other data needed for code approval. Some of these concerns were discussed in detail in the PIRT exercise performed by the GT-led IRP team.

6. Summary, Conclusions, and Path Forward

The workshop discussions together with the four PIRT panel meetings held prior to the workshop identified a large number of issues in fundamental data and gaps in modeling and simulations of FHRs in general as well as in the current tools. There are too many to enumerate or summarize here. As a result, a broad summary is provided in each modeling and simulation area.

There are large uncertainties in some of the cross sections of some materials specific to FHRs. Examples include thermal scattering kernel for graphite and salt. This type of uncertainty will be present in all current and future tools if not addressed. For accurate neutronic results, higher order transport (e.g., direct or hybrid stochastic deterministic transport) methods are needed. However, direct transport methods are currently computationally inefficient. Additionally, because of high core and fuel assembly heterogeneity deterministic transport methods require an accurate energy and spatial cross section condensation technique (an area of research).

Efficiency and accuracy of the low order transport methods such as diffusion theory depend on the robustness and efficiency of an accurate energy and spatial cross section condensation method. Experience indicates that use of whole-core stochastic methods for cross section condensation works well but must be done iteratively due to fuel depletion. However, inefficiency of such a method makes this methodology impractical for production/routine calculations, a key ingredient for licensing such a methodology. In short and this respect, development of an efficient and accurate method for generating multigroup spatially homogenized cross sections for both deterministic high and low order transport methods is an area of research.

Current neutronics codes such as SCALE and those in the NEAMS tool package can model FHR. However, in addition to the inefficiency issue, there are still code specific issues that require further development. For example, there is a lack of a robust method in current tools for transient calculations. Control rod modeling is an issue in pebble bed designs.

Libraries of fundamental thermo-physical property data for FHR are underdeveloped. There are often large uncertainties associated with properties such as thermal conductivity, viscosity, and thermal expansion in salts. Additionally, for these libraries to be fully complete and comprehensive for use in FHR calculations over all periods of reactor life and operation, they also need to include data for coolant salts with varying levels of impurities (e.g., due to corrosion).

Due to a lack of experimental data, there are phenomena associated with flowing coolant salt that are not well-understood. In order to accurately model these effects, there is a strong need for experimental data, including mixed-effect, separate-effect, and mixed-effect tests, such that the models can be validated.

Accident scenarios for FHR require coupled multiphysics tools much more than LWRs accident scenarios. To model effects such as salt freezing, and thus a coolant channel blockage, a materials-type code (to predict salt freezing patterns) would be coupled to a CFD code (to predict the new coolant flow pattern and the resulting T/H performance), which would in turn necessarily be coupled to a system-level code to predict reactor system response. For FHR licensing applications, it was concluded that robust multiphysics tools will be necessary.

From a materials standpoint, there is again the underlying problem of a lack of a fundamental data library for use in FHR calculations. Specifically, there is currently a strong need for standardized ways to measure redox of molten salts so that the results from different studies can be compared. Additionally, since salt impurities are the main reason for structural material corrosion, there is a need for reliable, standardized methods to quantify, and control, impurity levels in molten salts.

There currently exists very little modeling and simulation activity for modeling of structural material degradation in molten salts. Existing materials codes typically are used only for fuel calculations, and do not extend to FHR. Both as a standalone tool and as a tool for coupling in multiphysics calculations, having a tool to predict degradation of these structural materials would be a great asset in FHR analysis.

Each breakout session created a detailed list of areas of interest and research within their subject area. However, two major, unifying results were stated in all three sessions: the strong need for multiphysics tools, and the need for experimental data for validation purposes.

It is clear from these exercises that there is profound interest in this research area. The underlying conclusion from the PIRT panels, workshop, and thus this whitepaper, is that there is a number of gaps in current tools for FHR modeling and simulation. For use in design, analysis, and licensing of an FHR, the important gaps must be closed. It is demonstrated by the PIRT exercises and the workshop discussion that a broader organized push is needed to develop, verify, and validate these capabilities.

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- Pietro Avigni (GT) RELAP, TRACE, ANSYS Fluent, STAR-CCM+, OpenFOAM
- Kyle Ramey (GT) SERPENT

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Appendix A – Instrumentation Information

FLUX MEASUREMENT

Ionization Chambers and Fission Counters

Neutron flux monitoring is an important tool used for reactor control and safety functions. Spatial neutron flux profile awareness is necessary to safely maximize the reactor thermal output and signal deviations into flux tilting and shifting conditions. The technology of neutron flux detection has remained relatively unchanged for the past few decades, but signal processing methods have improved dramatically. New fission chamber designs have enabled single fission chambers to measure the entire working neutron flux range of power reactors [1]. Even with these advances, the placement of several neutron flux monitors, in addition to the plethora of other instrumentation will be challenging.

Self-Powered Neutron Flux Monitors

This class of neutron and gamma detectors produces a positive charge on one electrode by the emission of energetic electrons when exposed to radiation and do not need an external power supply for quantity measurement [3]. Major issues of the self-powered detectors are the vulnerability to spurious EMI and sensitivity burnup swing. The simplest neutron flux monitor can be as simple as a piece of standard television coaxial cable.

Current self-powered flux monitors could be upgraded for use in molten salt environments by the proper selection of high temperature, molten salt compatible materials. Nickel tubing, rhodium wire, and beaded ceramic insulator materials would be the most promising candidates. Candidate insulator materials would include, but are not limited to cerium dioxide, aluminum oxide, or scandium oxide.

Fiber-Optic, Cherenkov-Radiation Neutron Flux Monitor

The neutron flux monitor is derived from the Cherenkov radiation that is emitted from the fission daughter products, but it can be made more sensitive to neutrons by adding a short-lived beta emitter such as Cd or Gd to increase the Cherenkov signal due to the neutron flux [4]. Since the beta flux from fission is substantial, it would be simplest to use an uncoated, fiber bundle. The bundle would be sheathed in Hastelloy-N with a flexible lead bellows, also made from Hastelloy-N. The fibers themselves would be made from sapphire fiber coated with a micron-thick nickel clad. Error! Reference source not found. below is a conceptual drawing of the proposed detector with the dimensions exaggerated for clarity. The power profile is deduced by the difference in the Cherenkov signals between adjacent fibers. Sapphire is a durable material that is able to remain relatively transparent even under the harsh radiation environment of a nuclear reactor core, and should remain transparent up to 1019 n/cm3 [5], [6]. The defects should be able to be annealed out of the fiber at temperatures above 600ºC.

Modeling the fiber optic Cherenkov flux monitor has its problems rooted in the MCNP subroutines that model the physics of the creation and transport of Cherenkov light.

The transparent coolant also lends itself to the useful feature of using a lightpipe to transmit the information to a remote CCD that would collect high-resolution images of the reactor core at different points that could then be used to infer and reconstruct 3D internal power profiles. The TAMU team is currently investigating this technique using MCNP modeling and waterproof cameras at the TEES-NSC TRIGA reactor facility.

TEMPERATURE MEASUREMENT

Thermocouples, resistance temperature detectors (RTD) are widely used for temperature measurement. The most widely used material for RTDs is platinum, which limits it's use to 850ºC. Another disadvantage to their use in a potential FHR is its size and thermal inertia; they take time to respond and this is most prominent in gas temperature sensing situations.

Fiber-Bragg grating temperature sensors are the most mature fiber-based technology and commercially available fibers can withstand operational temperatures up to 900ºC [7]. The temperature range could potentially extend beyond the 900C range with the use of sapphire fibers, but the current limitation on length (<3m) and Bragg grating scribing methods require more research. Single point temperature measurements are feasible using hollow core fibers spliced at the end of the fiber to produce an optical cavity for temperature measurement.

PRESSURE MEASUREMENT

Absolute, Gauge, and Differential Pressure Measurement

Most pressure transducers use the deflection of a pressure sensing element to infer the pressure reading. The deflection can be measured using piezoresistive, piezoelectric, capacitive electromagnetic, resonant, and optical techniques. The diaphragm and measurement system can incorporate inherent errors due to hysteresis, temperature, and corrosion. The fiber optic techniques are best suited for the corrosive, high-radiation environments at higher temperatures [8].

Pressure Transducers

Current molten salt instrumentation for pressure relies upon the use of a pressure disk that separates the molten salt from a liquid NaK line that sends the pressure down a long tube to reduce the ultimate temperature to which the sensing element is exposed. This ultimately reduces the installation flexibility of the pressure sensor in a future FHR prototype.

The Fabry-Perot interferometer pressure transducer detects pressure disk deflections with sub-micron accuracy using the inherent length change measurements from multiple-bounce light-interference that is then transmitted via multimode optical fiber to a fringe pattern CCD sensor that translates the moving fringe pattern into pressure-disk deflections [9].

FLOW MEASUREMENT

Current molten salt system flow measurement is conducted using ultrasound in a dual diagonal crossflow arrangement. The mean flow velocity can be inferred by measuring the difference in transit time between upstream and downstream travelling sound waves. This measurement technique has the advantage of being completely unobtrusive to the flow path of the molten salt such that in the event of solidification, there are no delicate parts to break.

Flow measurement can be achieved from differential pressure measurement on flow through a venturi or ultrasonic methods. The pressure measurements can be performed by the fiber optic methods mentioned above or a suitably adapted ultrasonic transducer material.

Appendix B – Workshop Presentations

This appendix contains the slides from many of the presentations given at the workshop. Some have been very slightly modified and updated, but the core of the content is the same as what was presented.

AGENDA (March 8, 2017)

07:00am Continental breakfast and registration

Keynote Speakers

08:00 Welcome and introduction

08:20 Importance of modeling and simulation tools for advanced reactors – Dan Funk for Shane Johnson (DOE-NE) – *Slides have been updated*

Moderator – Dan Funk (DOE-NE)

08:30 Remarks by the National Technical Director for Molten Salt Reactors – Lou Qualls (ORNL) - ***No associated slides***

08:35 GAIN initiative updates – Rita Baranwal (GAIN)

08:45 EPRI / GAIN Modeling and Simulation (M&S) Initiative – Cristian Marciulescu (EPRI)

08:50 Kairos Power – Ed Blandford (Kairos Power) – ***Slides unavailable***

09:10 FHR Licensing – George Flanagan (ORNL)

M&S capabilities for AHTR & PB-FHR analysis

09:30 FHR & MSR modeling tools: past, present, and future – Lou Qualls (ORNL) – *Slides have been updated*

10:00 Break

Moderators – Paul Burke, Kyle Ramey

10:25 SCALE Enhancements for Advanced Reactor Analysis– Brad Rearden (ORNL)

10:55 An Introduction to NEAMS Workbench – Brad Rearden (ORNL)

11:25 A Multiscale FHR Modeling and Simulation Approach Employing NEAMS Tools – Rich Martineau (INL)

12:00 Lunch

01:30pm NEAMS/SHARP tool set – Elia Merzari (ANL) – ***Slides unavailable***

02:00 SAM tool set – Rui Hu (ANL) – ***Slides unavailable***

02:30 TRACE/PARCS tool set - Aaron Wysocki (ORNL)

03:00 Modelling of Advanced Reactor Concepts at CNL– Alex Levinsky (CNL)

03:30 Break

Moderators – Hemin Noorani, Giovanni Maronati

04:00 COMET tool set – Farzad Rahnema (GIT)

04:30 Current tools in use by Georgia Tech for AHTR analysis – Bojan Petrovic (GIT)

05:00 Current tools in use by UCB for PB-FHR analysis – Max Fratoni (UCB) – ***Slides unavailable***

05:30 Issues with modeling and simulation of tritium management in salt system – Pattrick Calderoni (INL)

Importance of modeling and simulation tools for advanced reactors

Dan Funk for Shane Johnson (DOE-NE) – *Slides have been updated*

U.S. DEPARTMENT OF ENERGY | Office of Nuclear Energy

Importance of Modeling and Simulation Tools to Advanced Reactors

R. Shane Johnson
Deputy Assistant Secretary
for Nuclear Technology Demonstration and Deployment
Office of Nuclear Energy

March 8, 2017

Office of Nuclear Energy Mission

In what part of NE's mission is the Advanced Modeling and Simulation Role Relevant and Significant?

Mission:

Advance nuclear power as a resource capable of meeting the Nation's clean energy, environmental, and national security needs by resolving technical, cost, safety, proliferation resistance, and security barriers through research, development, and demonstration.

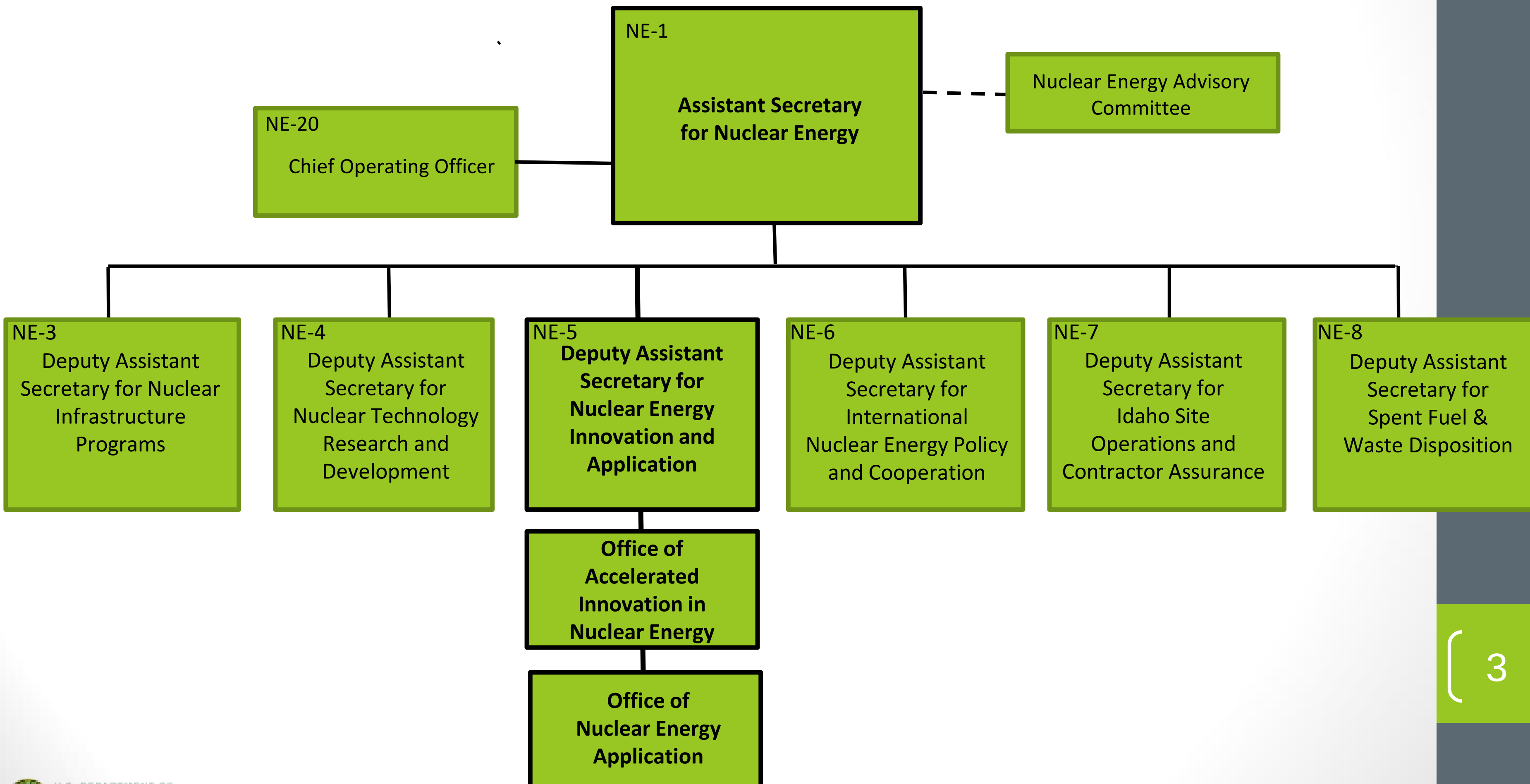
Mission Priority Areas:

- **Existing Nuclear Fleet** (LWR sustainability; Accident Tolerant Fuels)
- **Advanced Reactor Pipeline** (FOAK Advanced Small Modular Reactor, Versatile Advanced Test Reactor, Prototype Advanced Reactor, Advanced Reactor R&D, Nuclear Science User Facilities and Enabling Capabilities)
- **National Fuel Cycle Infrastructure** (Fuel Cycle R&D, Used Nuclear Fuel Disposition R&D)

U.S. DEPARTMENT OF ENERGY

Office of Nuclear Energy Organization

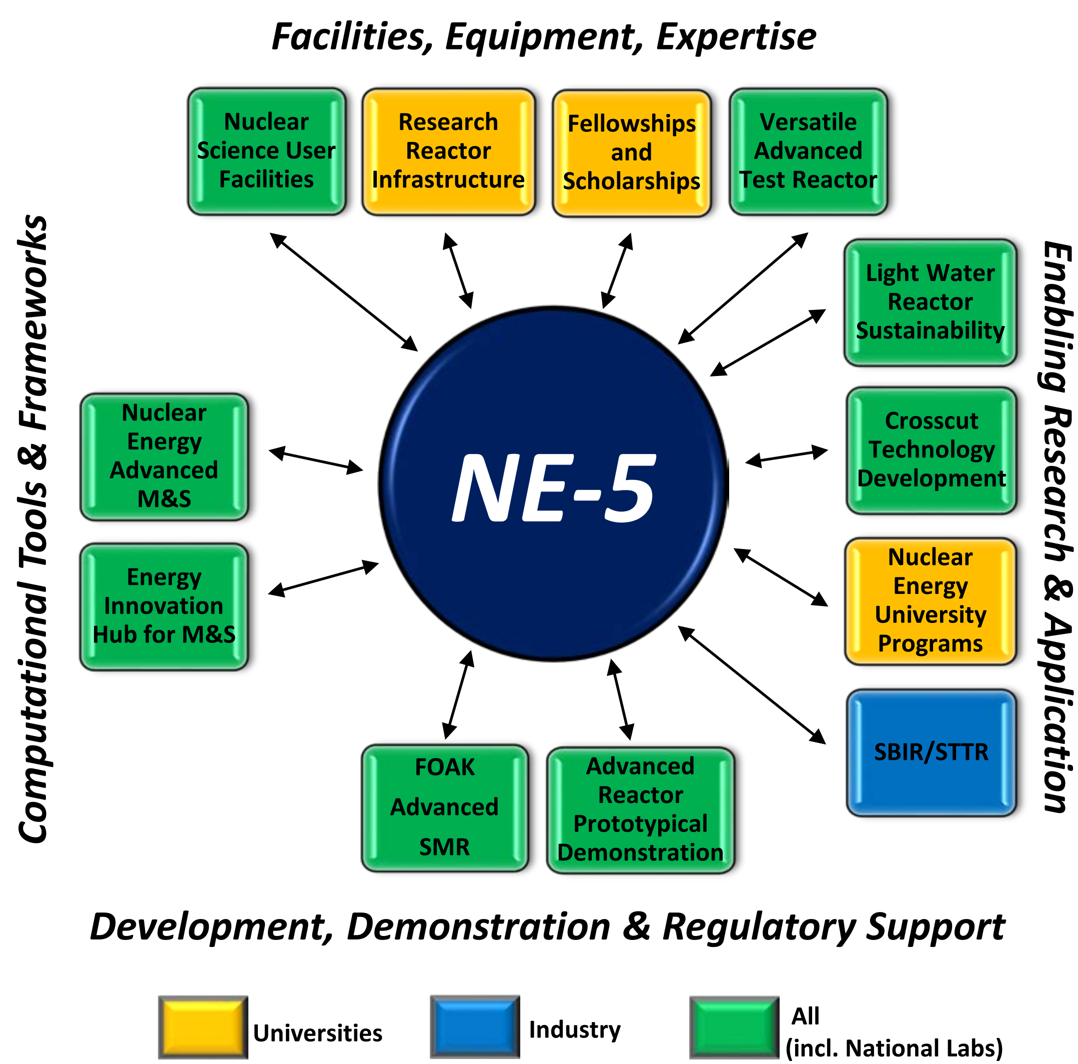
Where in NE are programs for developing and deploying advanced modeling and simulation tools managed?



U.S. DEPARTMENT OF ENERGY

Nuclear Energy Innovation and Application

Program Integration



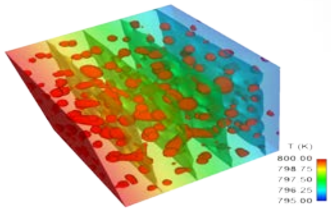
U.S. DEPARTMENT OF ENERGY

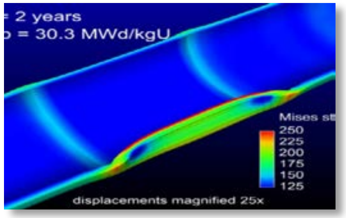
Computational Tools & Frameworks

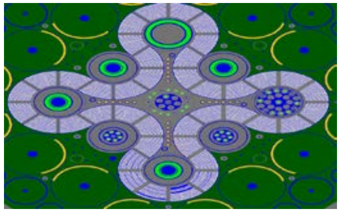
NE's Advanced Modeling & Simulation

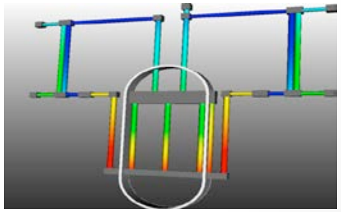
- **Develop state-of-the-art products** to support the existing LWR fleet and the next generation of reactor technologies (including small modular and non-light water designs)
  - Energy Innovation Hub for Modeling and Simulation (Hub)
  - Nuclear Energy Advanced Modeling and Simulation (NEAMS)
  - LWRS Work in RELAP-7 and other tools for Risk-Informed Safety Margin Characterization (RISMC)
  - Advanced Reactor Technology and Other R&D programs

- **Deploy broad range of advanced computational tools** to empower researchers/designers to accelerate the development and commercialization of new concepts, either to improve operation of the current fleet, or to optimize advanced reactor designs and ultimately deploy them for commercial use:
  - obtain fundamental insights that are unattainable through experiment alone; enhance experiments and analyses;
  - solve important development problems, reduce barriers (including time and cost) that are a high priority for the advanced reactor industry







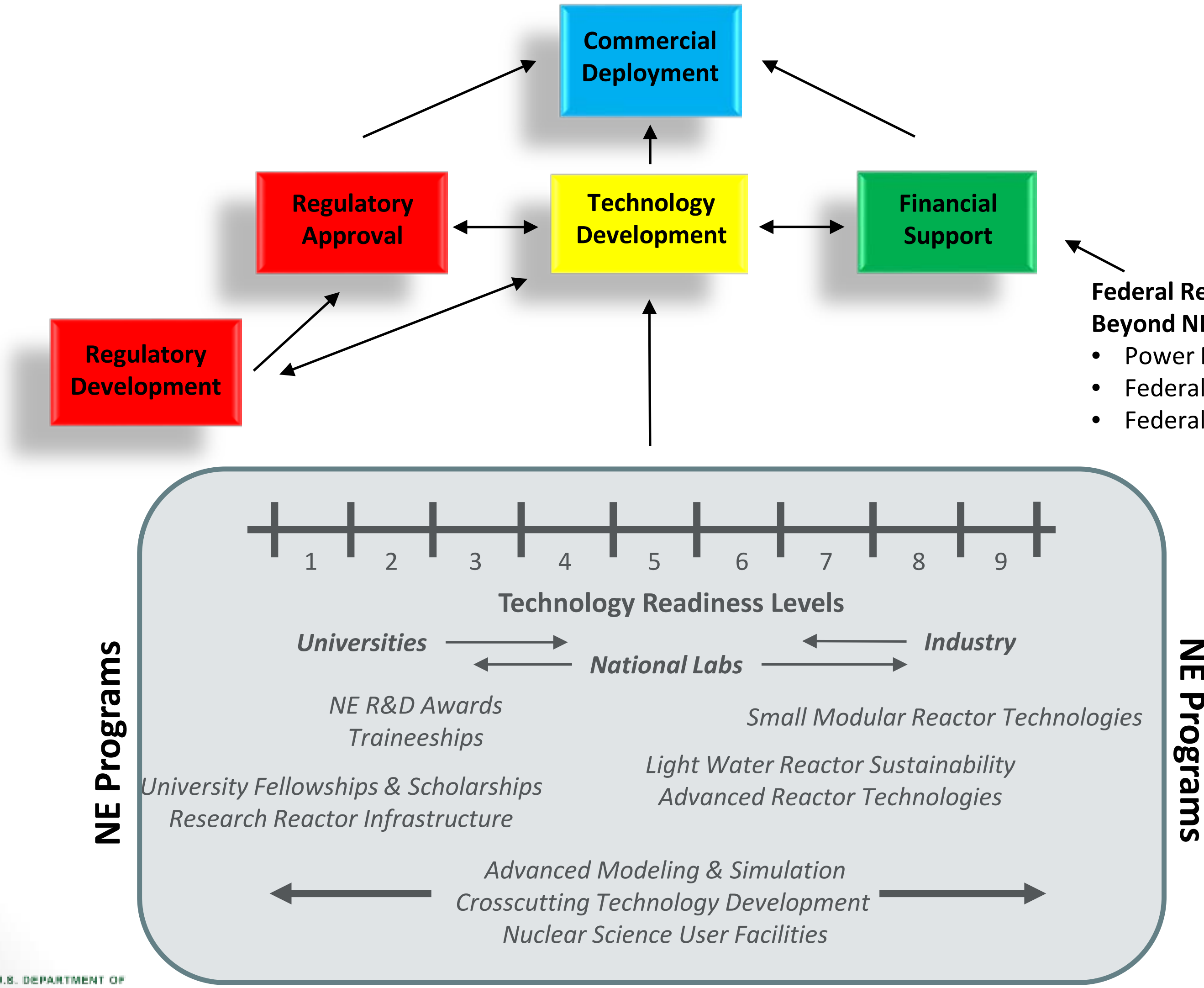


NE's Advanced Reactor Pipeline Strategy

How does Advanced Modeling and Simulation Fit in with this Strategy?

- ***Fully execute GAIN Initiative***
  - Ease the burden to Private Sector access to DOE assets
  - Institute "Single Point of Contact"
  - Standardize R&D agreements
- ***Demonstrate performance, reduce costs, and retire technical risks***
  - Partner through GAIN technology working groups to pursue industry-selected generic and design-specific R&D
- ***Support development of fuel cycle pathways***
- ***Support the establishment of a regulatory framework***
  - Work with GAIN technology working groups and NRC to advance the appropriate regulatory framework
- ***Maximize the effectiveness of public/private partnerships***
- ***Address human capital and workforce development needs***
  - Support university research and the development of next generation of nuclear professionals through vibrant university research infrastructure

Nuclear Energy Innovation and Application
Next Generation Reactor Deployment



Federal Resources Beyond NE's Authorities

- Power Purchase Agreements
- Federal Loan Guarantees
- Federal Land Use

Value Proposition

An **integrated and systematic approach** to
Nuclear Energy Innovation and Application
(***particularly deployment of advanced M&S tools***)
will allow the US Government, for the first time,
in collaboration with the private sector,
to serve as
an effective catalyst for the commercialization
of innovative nuclear technologies
to enable an expansion
of the US commercial nuclear industry.

Remarks by the National Technical Director for Molten Salt Reactors

Lou Qualls (ORNL) - ***<u>No associated slides</u>***

GAIN initiative updates

Rita Baranwal (GAIN)

GAIN

Gateway for Accelerated Innovation in Nuclear

Dr. Rita Baranwal
Director, GAIN

March 8, 2017

Idaho National Laboratory

Oak Ridge National Laboratory

Argonne National Laboratory

5 things we'll talk about today

- ***Safety Brief***
- ***What is GAIN?***
- ***Recent Successes***
- ***Future Activities***

What is the GAIN initiative?

Gateway for Accelerated Innovation in Nuclear

What are the issues?

- Time to market is too long
- Facilities needed for RD&D are expensive
- Capabilities at government sites have not been easily accessible
- Technology readiness levels vary
- Some innovators require assistance with regulatory process

What do we need to do?

- Provide nuclear innovators and investors with single point of access into DOE complex
- Provide focused research opportunities and dedicated industry engagement
- Expand upon DOE's work with Nuclear Regulatory Commission (NRC)

What is the DOE initiative?

GAIN
Gateway for Accelerated Innovation in Nuclear

- Public-private partnership, dedicated to **accelerating** innovative nuclear energy technologies' **time to market**

DOE recognizes the magnitude of the need, the associated sense of urgency and the benefits of a strong and agile public-private partnership in achieving the national goals.

GAIN
Gateway for Accelerated Innovation in Nuclear

GAIN Vision

By 2030,

The U.S. nuclear industry is equipped to lead the world in deployment of innovative nuclear technologies to supply urgently needed abundant clean energy both domestically and globally.

GAIN is …

A public-private partnership framework aimed at rapid and cost-effective development of innovative nuclear energy technologies toward market readiness.

GAIN

Gateway for Accelerated Innovation in Nuclear

GAIN Mission

Mission:

As the organizing principle for the relevant DOE-NE programs, provide the nuclear energy industry with access to technical, regulatory and financial support necessary to move innovative nuclear energy technologies toward commercialization in an accelerated and cost-effective fashion.

GAIN is …

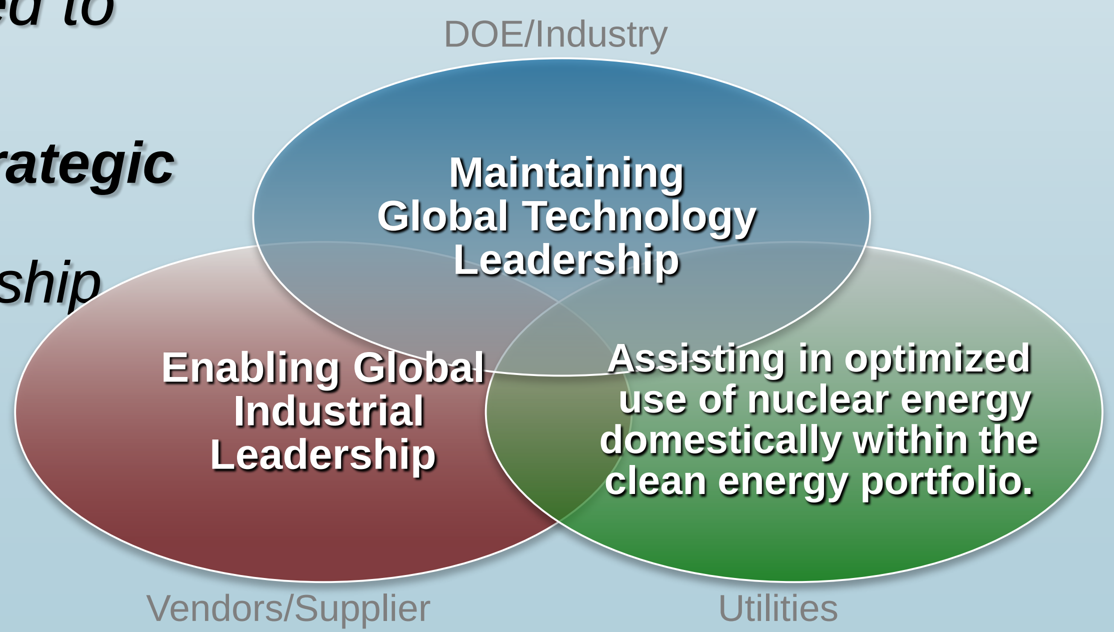
The organizing principle for the relevant, federally-funded nuclear energy RD&D programs.

GAIN Initiative: Simultaneous Achievement of Three Strategic Goals

1. *National and global demand for nuclear energy is increasing and U.S. global leadership is eroding*
2. *There is a **sense of urgency** with respect to the deployment of the innovative nuclear energy technologies*
3. *An effective **private-public partnership** is required to achieve the goals*

*Achievement of **GAIN's Strategic Goals** will bridge the gap between technology leadership and industrial leadership*

STRATEGIC GOALS



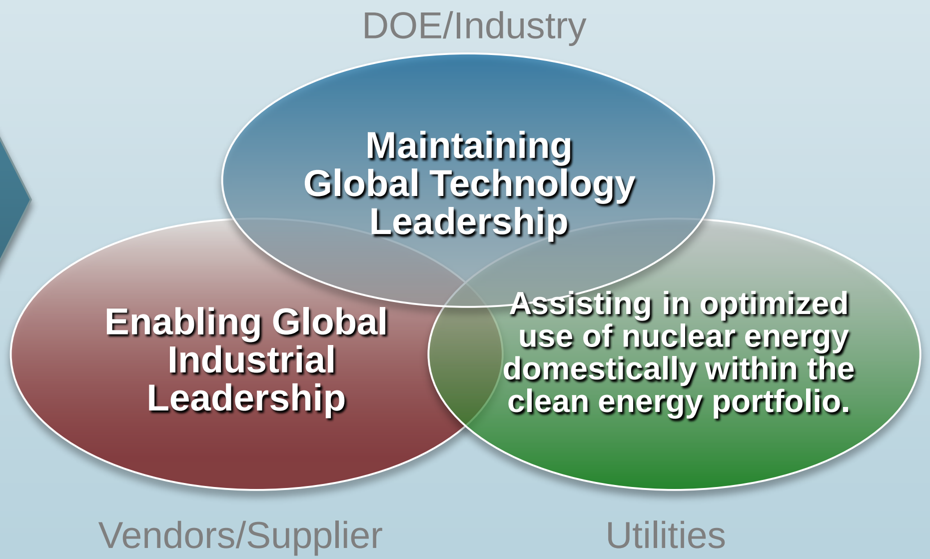
GAIN

GAIN Explores New Model for Faster and More Cost-Effective Innovation Cycle for Nuclear Energy

DOE, Vendors and Utilities

Private-Public Partnership Model: Integrated approach to development, demonstration and deployment of innovative nuclear technologies for faster, more cost-effective innovation cycle.

STRATEGIC GOALS



GAIN

GAIN Organization

Director: Rita Baranwal
Deputy Director: Doug Crawford

Executive Advisory Committee

- Neil Wilmshurst, EPRI – Chair
- Dale Klein, University of Texas
- Maria Korsnick, NEI
- Steve Kuczynski, SNC
- Paul Kearns, ANL
- Thom Mason, ORNL
- Chris Mowry, ARC
- Mark Peters, INL
- Ray Rothrock

Integration Working Group
Chair: Hussein Khalil

Expert oversight of GAIN execution strategy
And high-level documents/deliverables.

Coordinator
Lori Braase

- Administrator
- Communications
- Business Manager

Technical Interface
John Jackson

- Project Manager
- Lab Technical POCs

Idaho National Laboratory
Oak Ridge National Laboratory
Argonne National Laboratory

GAIN

GAIN:
Organizing Principle for DOE-NE RD&D Programs Through Comprehensive Systems Analysis

Modeling & Simulation
HPC Infrastructure

Validated software

M&S expertise

Crosscutting Design Support
Nuclear Hybrid Energy

Nuclear Cyber Security

Digital I&C/ Human Factors

NRC Interface
Licensing framework

Gradual risk reduction

Licensing support Expertise

Base Reactor and Fuel Cycle R&D Programs
Advanced Fuel Cycles

Advanced Reactors

LW-based Reactors

Experimentation
Infrastructure

Instrumentation and sensors

Manufacturing Expertise

M&S Capabilities

Knowledge & Validation Center

Experimental Capabilities

– GAIN –
Industry and investor access to DOE capabilities and expertise

Activities to Date

GAIN Operations

- *Established small, agile organization*
- *Issued GAIN Execution Plan*
- *Issued Technology Specific Workshops Summary Report*
- *Implemented Standard CRADAs/TAPAs for NE vouchers*

GAIN Outreach

- *Presented GAIN to multiple conferences/meetings to solicit input from stakeholders*
- *Organized 3 Technology Specific Workshops (with NEI and EPRI) to solicit input on private-sector R&D needs for DOE-NE R&D program*
- *Conducted 2 Modeling & Simulation workshops*
  - *Model for additional future workshops*

GAIN Support of Private Sector

- Awarded $2M USD to developers in pilot NE Voucher Program
- Initiated industry-led, laboratory-supported expert group for advanced reactor licensing framework development
- Submitted FY 2018-2022 DOE-NE RD&D funding request

GAIN
Gateway for Accelerated Innovation in Nuclear

Early Success: NE Voucher Program

- ***Eight small businesses were awarded for the 2016 pilot (~$2M total)***
- ***Goal:*** *Assist small businesses in accelerating development and deployment of innovative nuclear technologies by granting access to extensive nuclear research capabilities available at DOE's national laboratories and Nuclear Science User Facilities (NSUF) partners*
- ***2017 voucher call will award $4M***

NE Voucher recipients	Proposal	Partner Facility
Creare LLC Hanover, NH	Investigation of Materials for Continuous Casting of Metallic Nuclear Fuel	Idaho National Laboratory
Columbia Basin Consulting Group, LLC Kennewick, WA	Lead-Bismuth Small Modular Reactor (SMR) Licensing Development	Pacific Northwest National Laboratory
Terrestrial Energy USA Ltd. New York, NY	Verification of Molten-Salt Properties at High Temperatures	Argonne National Laboratory
Transatomic Power Corporation Cambridge, MA	Optimization and Assessment of the Neutronics and Fuel Cycle Performance of the Transatomic Power Molten Salt Reactor Design	Oak Ridge National Laboratory
Ceramic Tubular Products Rockville, MD	Robust Silicon Carbide Cladding for LWR Application - Corrosion and Irradiation Proof Test of Low Cost Innovations in MIT Research Reactor	Massachusetts Institute of Technology
Oklo Inc. Sunnyvale, CA	Legacy Metal Fuel Data Exploration for Commercial Scale-Up	Argonne National Laboratory/Idaho National Laboratory
CompRex, LLC De Pere, WI	High Efficiency Heat Exchanger for High Temperature and High Pressure Applications	Argonne National Laboratory
BgtL LLC Laramie, WY	High efficiency and low cost thermal energy storage system	Argonne National Laboratory

2017 GAIN TECHNICAL WORKING GROUPS (TWGs)

Molten Salt Reactor	
Elysium Industries	Boston, MA 02111
Flibe Energy	Huntsville, AL 35806
Southern Company	Birmingham, AL 35291
TerraPower LLC	Bellevue, WA 98005
Terrestrial Energy USA Ltd.	New York, NY 10155
Transatomic Power Corp.	Cambridge, MA 02142
High Temp Gas Reactor	
AREVA NP Inc.	Lynchburg, VA 24501
BWXTechnology	Lynchburg, VA 24504
Duke Energy	Charlotte, NC 28202
StarCore Nuclear Co.	Canada
X-Energy LLC	Greenbelt, MD 20770
Fast Reactor	
Advanced Reactor Concepts	Chevy Chase, MD 20815
Columbia Basin Consulting Group	Kennewick, WA 99336
Duke Energy	Charlotte, NC 28202
Elysium Industries	Boston, MA 02111
Exelon Corporation	Chicago, IL 60603
General Atomics	San Diego, CA 92121-1122
General Electric-Hitachi	Wilmington, NC 28401
OKLO Inc.	Sunnyvale, CA 94089-1007
Southern Company	Birmingham, AL 35291
Terra Power	Bellevue, WA 98005
Westinghouse	Cranberry Township, PA 16066

GAIN

Technology-Specific Workshops: Collaboration

Formation of Industry-Led Technology Working Groups (TWG)

- *Initial meetings held in September 2016*
- *Molten Salt Reactor*
- *Fast Reactor*
- *High Temperature Gas Reactor*

Roles and Responsibilities

- **EPRI:** engage with subject matter experts & stakeholders
  - Define gaps in M&S code development and V&V for design and licensing for advanced reactor technologies
- **NEI:** facilitate and coordinate activities of TWGs with those of NEI Advanced Reactor Working Group (ARWG)
  - Coordinate with GAIN and EPRI to support working groups
  - Work with industry, DOE, and NRC to understand issues associated with obtaining 5% < enriched uranium < 20%

EPRI | ELECTRIC POWER RESEARCH INSTITUTE

NEI NUCLEAR ENERGY INSTITUTE

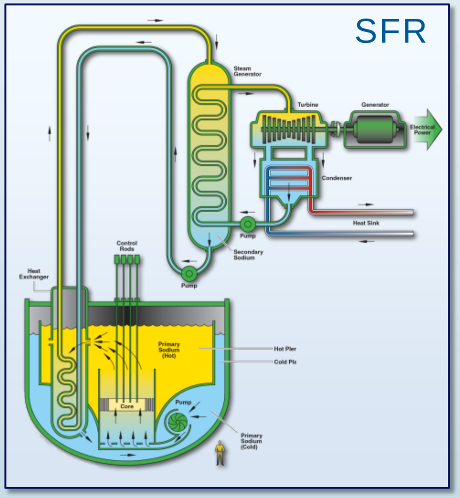
Technology-Specific Workshops:
High-priority recommendations to DOE on cross-cutting RD&D

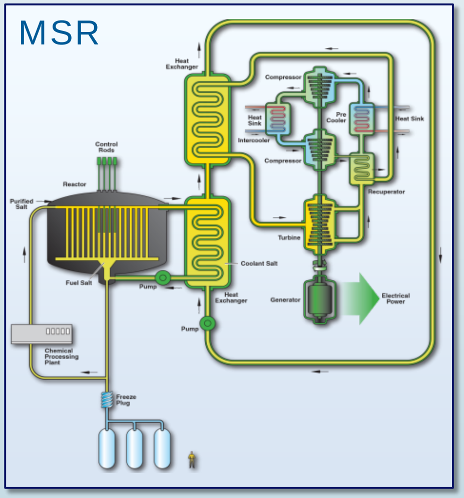
- ***Access to Applied Technology (AT) documents***
  - *Create database of AT-marked documents*
  - *Streamline access to AT documents, removing AT designation where appropriate*
- ***M&S Code Development and V&V for Design & Licensing***
  - *Describe DOE-NE's advanced M&S tools*
  - *Develop plans for additional code development to address gaps*
  - *Develop joint strategy with stakeholders for V&V of advanced tools*
  - *Develop joint strategy with NRC for V&V and usage of advanced tools for licensing analyses*
- ***Advanced Reactors Licensing Framework***
  - *Accelerate joint work with NRC for advanced reactor licensing*
    - *General design criteria*
    - *Gradual reduction of licensing risk*
    - *Risk-informed and performance-based licensing strategy*

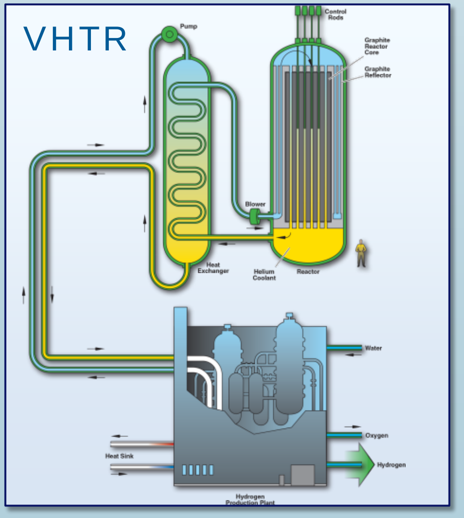
GAIN
Gateway for Accelerated Innovation in Nuclear

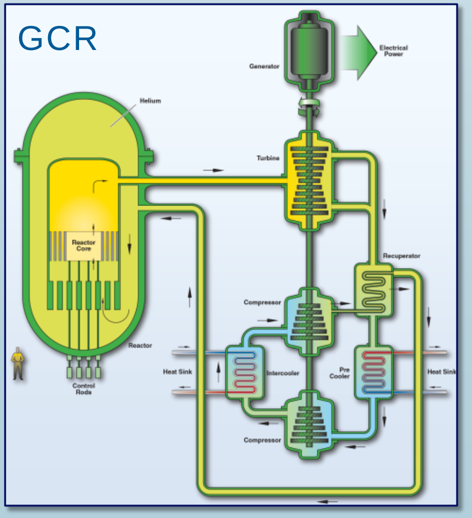
Technology-Specific Workshops:
High-priority recommendations to DOE on design-specific technology

- ***Molten Salt Reactor Technology***
  - *Identify alternatives to critical-system demonstration for meeting all identified data needs using different and simpler options*
- ***Fast Reactor Technology***
  - *Complete options and requirements assessment for domestic fast spectrum test reactor*
- ***High Temperature Gas Reactor Technology***
  - *Complete on-going TRISO fuel and graphite qualification program*









GAIN

Future Activities 2017

From U.S. Senate Committee on Energy and Natural Resources January 19, 2017 Department of Energy Secretary Nomination Hearing: Responses to Questions for the Record:

Q: I'm interested to hear, what you will do, if confirmed, to work with the bipartisan group of Senators to continue to ensure that DOE is equipped with adequate funding to continue researching and developing these advanced reactor designs.

A: "Nuclear energy is a critical component of America's energy future, and entrepreneurs are developing promising new technologies that could truly spur a renaissance in the United States and around the world. DOE, through the National Labs complex, maintains unique government facilities that can assist in the development of advanced nuclear energy technologies. ***The GAIN initiative provides the potential for public-private partnerships to thrive in the future. If I am confirmed, I look forward to learning more about how DOE can support advanced nuclear reactor development."***

GAIN
Gateway for Accelerated Innovation in Nuclear

Future Activities 2017

- ***Identify/develop Streamlined Contracting Process***
  - *Streamline and tailor DOE contracting mechanisms to meet GAIN goals*
  - *Identify candidate project and participants for multi-party CRADA (contracting pilot)*
  - *Identify new partnership mechanisms*
- ***NE Voucher Activities***
  - *Second NE Voucher Call: February 9, 2017*
- ***Support development of a flexible fast spectrum test reactor options study based on industry requirements***
- ***Workshops:***
  - *TREAT/Fuel Safety Research: May 1-4, 2017 at INL*
  - *Instrumentation &Controls*
  - *Advanced Manufacturing*
- ***Develop database of historical advanced-reactor documents to support knowledge transfer; facilitate access to key documents through OSTI***
- ***Create industry-accessible electronic catalog for modeling and simulation applications***

GAIN
Gateway for Accelerated Innovation in Nuclear

Summary

- ***GAIN*** *is establishing a public-private partnership to achieve* ***3 strategic goals***
- ***GAIN*** *is being implemented as the* ***organizing principle*** *for relevant DOE programs*
- ***Future efforts*** *intend to improve* ***GAIN effectiveness*** *and* ***impact***

GAIN
Gateway for Accelerated Innovation in Nuclear

"Those who say
it cannot be done
should not interrupt
those who are doing it."

- Chinese Proverb

GAIN

http://gain.inl.gov

Twitter @GAINnuclear

Facebook: @GAIN – Gateway for Accelerated Innovation in Nuclear

EPRI / GAIN Modeling and Simulation (M&S) Initiative

Cristian Marciulescu (EPRI)

EPRI / GAIN Modeling and Simulation (M&S) Initiative

Cristian Marciulescu
Principal Technical Leader

FHR Workshop
Georgia Institute of Technology
March 8th, 2017

EPRI / GAIN M&S Initiative

- Gateway for Accelerated Innovation in Nuclear (GAIN) was established to provide the nuclear community with a single point of access to the broad range of capabilities across the DOE/laboratory complex

- **July 2016** - EPRI (with NEI and GAIN) hosted three technology-centric workshops, to focus, discuss and collect feedback on specific developer RD&D needs

- Modeling and simulation (M&S) capabilities to support design and licensing was identified as a top cross-cutting need

- EPRI's action: engage with subject matter experts and stakeholders to define gaps and to coordinate efforts to address these gaps

EPRI / GAIN Modeling and Simulation (M&S) Initiative

- **December 12, 2016** – EPRI/NEI/GAIN Workshop on M&S Needs
  – NEI offices in Washington, D.C.
  – Advanced reactors developers presented their common M&S needs to GAIN, DOE and national lab representatives
  – GAIN and national labs agreed to prepare a gap analysis relative to existing software codes developed and maintained under DOE programs

- **January 24-25, 2017** – EPRI hosted Second GAIN M&S Workshop in Charlotte
  – direct interaction between advanced reactor developers (12 unique companies were represented) and M&S experts from the U.S. national laboratories (35 participants)
  – presentation of results from the DOE/GAIN/national laboratory M&S gap analysis
  – discussion of potential paths forward for addressing priority gaps

- A DOE/GAIN summary report will document gap analysis and recommendations

Kairos Power

Ed Blandford (Kairos Power) – ***<u>Slides unavailable</u>***

FHR Licensing

George Flanagan (ORNL)

FHR Licensing

Presented by:

George Flanagan
Reactor & Nuclear Systems Division
Oak Ridge National Laboratory
flanagangf@ornl.gov, (865) 574-8541

For the:

Workshop on Tools for Modeling and Simulation for FHRs-Gaps and Development Needs
Georgia Institute of Technology, Atlanta, GA

March 8, 2017

OAK RIDGE National Laboratory

Content of the Presentation

- NRC/DOE / industry initiatives
- NRC strategic plan and implementation action plans related to codes and models

Advanced Reactor Licensing is Being Addressed by DOE, NRC, and Industry (NEI)

- NRC has issued a draft regulatory guide DG 1330 which contains advanced reactor design criteria, sodium fast reactor (SFR) design criteria and modular high temperature reactor (mHTGR) design criteria
  - Similar but not the same as the DOE team recommendation
  - Does not contain FHR criteria but ANS 20.1 is intended to provide criteria for consideration by NRC for endorsement
- DOE has initiated work on revising NUREG 800 (Standard Review Plan) to accommodate SFR and mHTGR
- DOE had initiated a pilot study of consensus standards that may need to be changed in order to accommodate advanced reactors
- There are a number of other initiatives related to advanced reactor licensing improvements under way, however, no clear path has been identified
- DOE has begun work on a technology neutral licensing framework implementation plan which encompasses some aspects of ANS 53.1 (long term item >10 years under NRC strategy # 3) – next slide
- Industry has drafted several bills, now pending in Congress, requiring NRC to develop an improved licensing process for advanced reactors

NRC has Published a Strategic Plan and Near Term Implementation Action Plans

- Strategy 1: Acquire knowledge and technical skills to perform non-LWR review
- Strategy 2: Acquire/develop computer codes and tools to perform non-LWR review
- Strategy 3: Develop guidance for flexible non-LWR reviews with in bounds of existing regulations including conceptual design and staged licensing reviews
- Strategy 4: Facilitate industry codes and standards
- Strategy 5: Address policy issues that impact reviews, siting, permitting etc.
- Strategy 6: Address structured process for communication to stakeholders

Strategy 2 has a Number of Actions in the Implementation Action Plan

- Functional areas to be addressed
  - Reactor kinetics, physics, and criticality
  - Fuel performance
  - Thermal-fluids
  - Severe accidents
  - Consequence analysis
  - Materials and component integrity
- LWR tools are deemed adequate for other areas such as seismic, structural, human reliability, and PRA
- NRC has indicated that to the extent possible they will rely on industrial developed codes instead of developing their own
  - NRC will need to be involved in the development in order to assure quality and applicability

Reactor Physics and Kinetics: NRC Will Perform a Functional Needs Assessment of SCALE and PARCS for Applicability to Non-LWRs

- Ten steps were identified
  1. Functional needs of codes
  2. Conditions and transients to be modeled
  3. Important phenomena that must be modeled (PIRT)
  4. Assessment of existing reactor core and analysis and criticality safety capabilities
  5. Identification of phenomenological gaps
  6. Identify the data needed to validate codes
  7. Collect and organize the data
  8. Develop codes
  9. Performance tests to obtain additional data
  10. Validation of the codes with the data

For FHRs, General Needs Were Identified

- Need for higher order stochastic and deterministic transport methods in order to fully capture the multiple heterogeneous nature of fuel
  - Multi-group cross sections structure to incorporate geometry, burnable absorbers, control rods and energy spectrum
  - Homogenization and de-homogenization of the fuel
  - Characterization of spatial transport mesh within the assembly
  - Scattering kernel within the graphite
- Nuclear data for graphite and FLiBe

Experimental Data Needs for FHR Were Identified

- Absorption cross sections for graphite and FLiBe
- Cross sections for impurities in graphite and FLiBe
- Scattering kernel kinematics for graphite and FLiBe

Other Information Modeling Needs Identified for FHRs

- Tritium transport through primary and secondary loops
- Ability to estimate the dose to workers

Fuel Performance Code Assessment (Not Directly Addressed for FHRs)

- Adapted from HTGR approach
  - Identify experimental data needs
  - Evaluate transport codes such as MELCOR for use in fission product transport analysis
  - Evaluate the usefulness of HTGR TRISO fuel experimental data
  - Determine the need for additional data

OAK RIDGE National Laboratory

Thermal-Fluid Modeling (Not Directly Addressed for FHRs)

- Evaluate the codes that have been developed for the HTGR
  - Address both prismatic and pebble configurations
  - Adapt PARCS for use in FHR environment
  - Need something equivalent to AGREE for FHRs to model heat transfer
  - TRACE has been adapted for use in MSRs, could be adapted for FHRs
  - Adapt CFD codes such as FLUENT or STAR-CCM+ for local detail flow analysis
  - Adapt MELCOR for global behavior and accident progression
  - Adapt features of GRSAC for accidents in FHRs
- Examine non-core issues using adaptations of SFR codes (intermediate loops)

Severe Accident Modeling (Not Directly Addressed for FHRs)

- Intent is to use modified MELCOR code for all three reactor types
  - Specific gaps were identified in the mHTGR PIRT most applicable to FHRs
    - Extended fission product release models for TRISO fuel
    - Graphite oxidation models
    - Update materials properties
    - Passive residual decay heat removal model (RCCS, DRACs or other)
    - Graphite dust (may not be as significant as for HTGR)
    - Improved numerics to address longer response times
    - Possible improvements in fission product transport and deposition

Offsite Consequence Analysis (Not Directly Addressed for FHRs)

- Intent is to use the MACCS code
  - Modifications are needed to address
    - Different radionuclides and chemical forms
    - Environmental release pathways (may need to address pathways than airborne plumes)
    - Atmospheric transport and dispersion (ATD) may need to be modified for more urban settings)
    - Chemical hazards (not currently in MACCS, additional models may be needed to account for any hazardous material released in and FHR)

Structural Integrity Codes (Not Directly Addressed for FHRs)

- In general, the program will need detailed information on operational environments such a temperatures and radiation levels to determine the applicability of existing codes.
- ASME Section III, Division 5 high temperature materials will address additional failure mechanisms and failure modes which will need to be introduced into the current models or new models will need to be developed.

Conclusion

- NRC's plan for codes is to use existing codes where possible minimizing development costs
- Any new codes will need adequate V&V and benchmarking
  - Experiments (separate effects testing and integral effects testing) along with scaling will be required
  - Lack of operational data will likely require more V&V than currently required for LWRs
  - Industrially developed codes may be used in lieu of NRC developed confirmatory codes, if NRC is allowed to follow or participate in the development of the code
- No indication that M&S codes will reduce the need for experiments in the current strategic plan action plans (next 5 years)
  - Use of M&S is addressed in the plan as an additional tool for consideration in the future

FHR & MSR modeling tools: past, present, and future

Lou Qualls (ORNL) – *Slides have been updated*

MSR Modeling Tools: Past, Present and Future

Brian Ade, ORNL
Reactor & Nuclear Systems Division

B. Betzler, A. Wysocki, J. Rader, S. Greenwood, B Ade, M. Jessee, G. Ilas, L. Qualls

For the:
Advanced Reactor Working Group Modeling & Simulation Workshop
EPRI, Charlotte, NC

January 24-25, 2017

MSR Modeling and Simulation Issues

- MSR technologies consist of both **fast** and **thermal** neutron spectrum reactors with a variety of potential **chloride** or **fluoride** salts.

- Need modern **modeling and simulation tools** and **data** to begin **validation**
  - Integral benchmarks for reactor physics
  - Thermal hydraulics
  - Material properties and response models
  - Coolant/fuel/structure chemistry/corrosion

- Molten salt-fueled reactors are unique due to the **convection of delayed neutron precursors** and the **transit times** of the fuel through the core and the remainder of the primary loop.
  - Delayed neutron precursor drift
  - Simplified models accurately replicated MSRE dynamics and are being recaptured

The successful operation of the Molten Salt Experimental Reactor Experiment provides evidence of the predictable nature of MSRs, some reactor physics benchmarking data, and evidence of technology gaps to be overcome for commercial deployment.

MSR Modeling Activities

- **Emphasis on tools for deployment**
  - ***Understand*** how a system will perform and evaluate it in order to make business decisions
  - ***Design*** (continuing the evaluation process)
  - ***Licensing*** (design specific models and tools)

- **Existing tools are available for immediate use**
  - Additional tools can be easily adapted for MSR evaluation (i.e., add proper salt properties)
- **Several initiatives recently started for the ATDR FHR-DR Point Design activity**
  - Continued development of these codes
  - Identification of gaps
- **New initiatives have begun**
  - Leveraging experience with other reactor types for MSR application

Modeling and Simulation Activities

- Establish ***functional requirements*** for M&S tools
- Define ***suite of tools*** to be developed
- Generate quality ***input data***
- Find or generate necessary ***validation data***
- Apply models to ***specific design*** cases

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What do you need to know?

Material and Material Systems Models; physical properties, irradiation response models, corrosion models

- What is your coolant?
  - What is “really” in your coolant over the course of the reactor lifetime?
- What is your structural material and how does it perform over it’s expected lifetime?
  - What can be it counted on to do at the worst possible time?
- What are the lifecycles for fission and activation products?

Production and loss terms from nuclear interactions, chemical interactions, and loss across the boundaries

- What performance do you need to make an economically viable system?
- How does that system behave?

Neutronics, thermal-hydraulics, dynamic system performance, activation areas and intensities

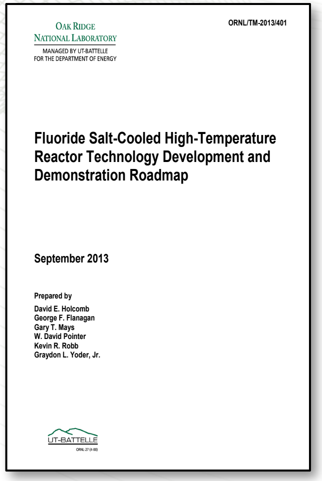
- What design-specific normal, off-normal, and accident scenarios do you need to consider to meet licensing requirements?
- What systems have to be developed to accommodate all anticipated scenarios?

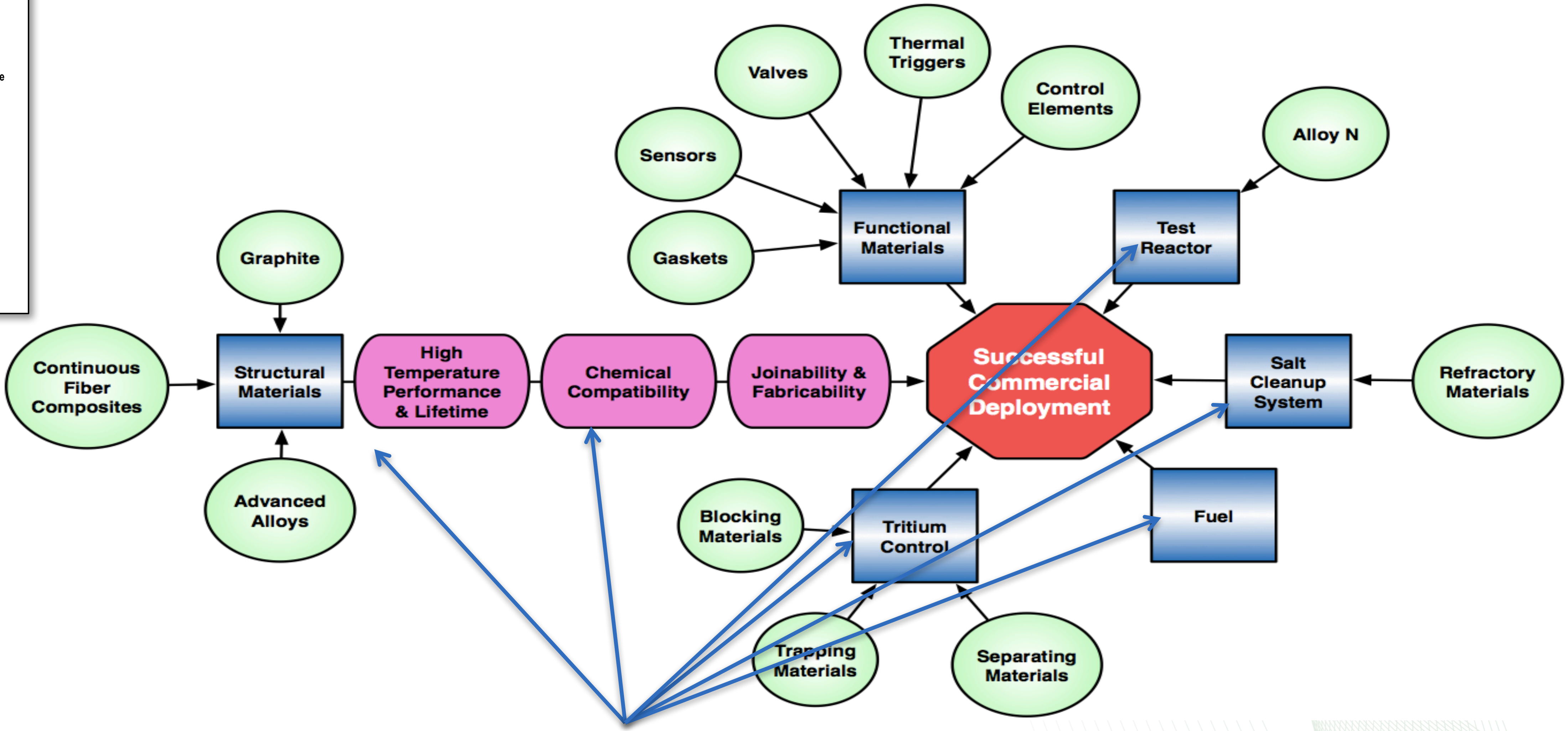
Chemistry control, passive safety system response

- What data do you need to support your case?

Severe accident analysis

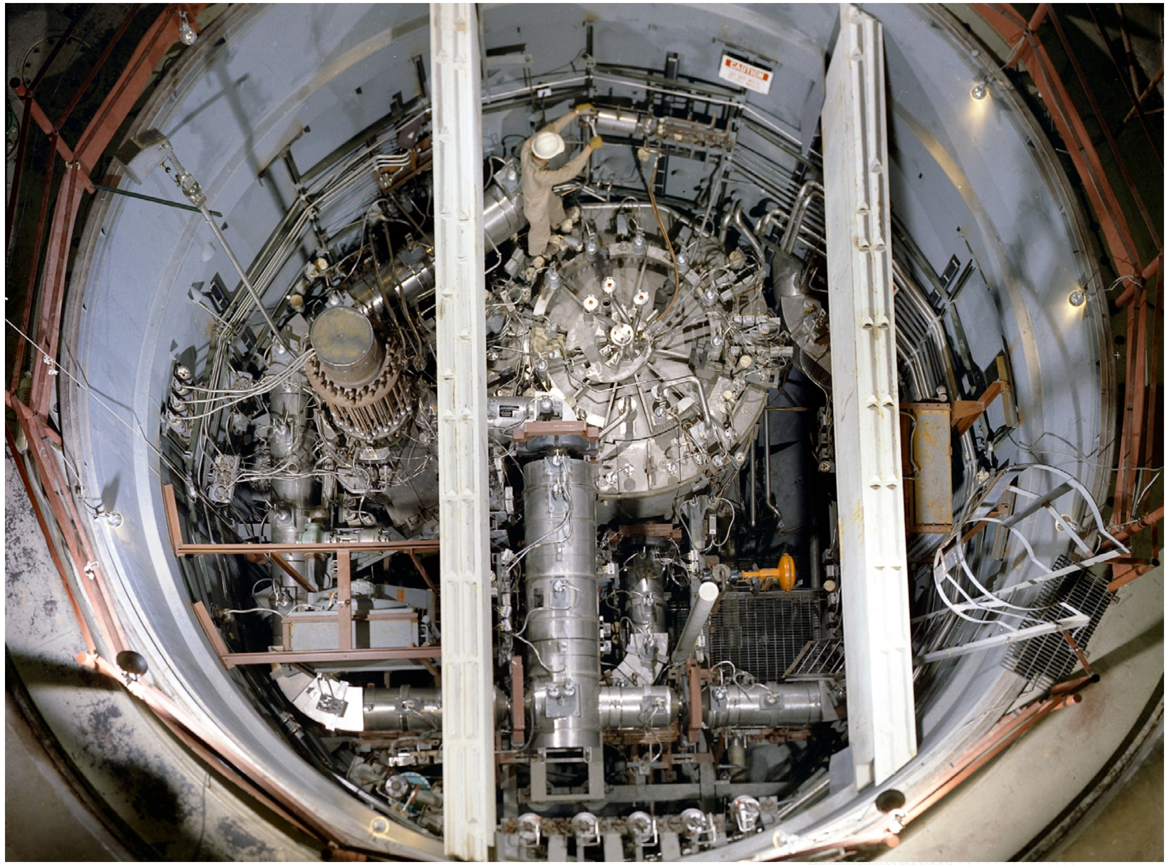
Development Needs Addressed by Coupled R&D and M&S





New or better models needed

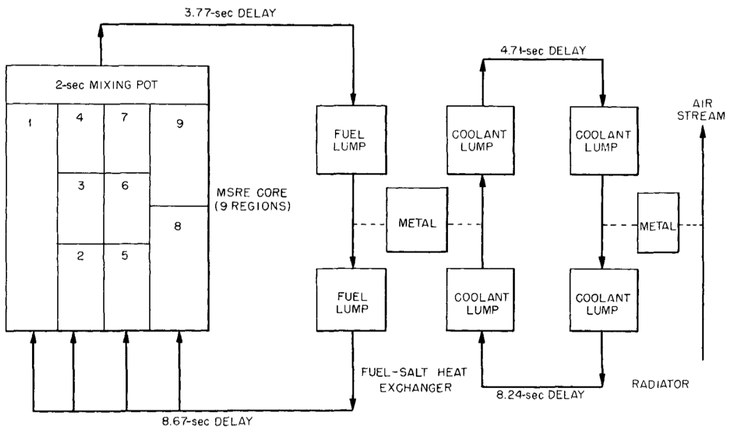
Molten Salt Reactor Experiment



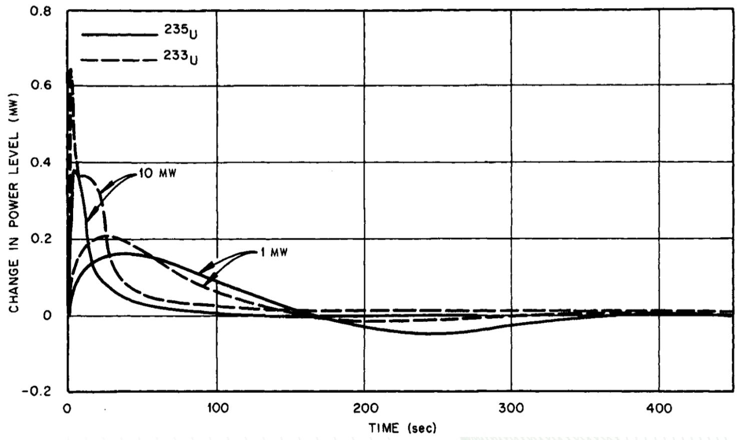
MSR Plant Dynamic System Model

(Jordan Rader, raderjd@ornl.gov)

- Based on Molten Salt Reactor Experiment Models
  - Transient responses verified by reactor operation
  - Modelica-based platform consistent with ORNL TRANSFORM M&S Tool
    - Reactor kinetics
    - Heat transfer
    - Fluid flow
- Can be easily coupled to power conversion systems or heat rejection systems within TRANSFORM
- TRANSFORM runs quickly on a single workstation
- Results compare well with MSRE measured data



Schematic representation of MSRE reference model



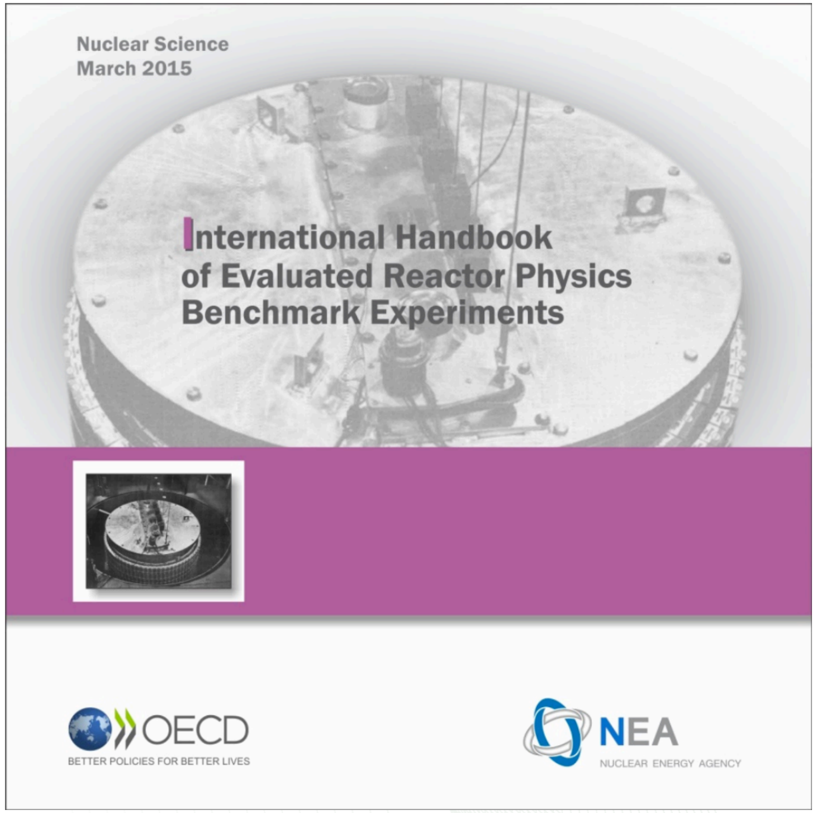
MSRE transient response to a +0.01% $\delta\rho$ step reactivity input when operating at 1 and 10 MW.

Kerlin et al, Theoretical Dynamics Analysis of the Molten-Salt Reactor Experiment, *Nuclear Technology*, 1971.

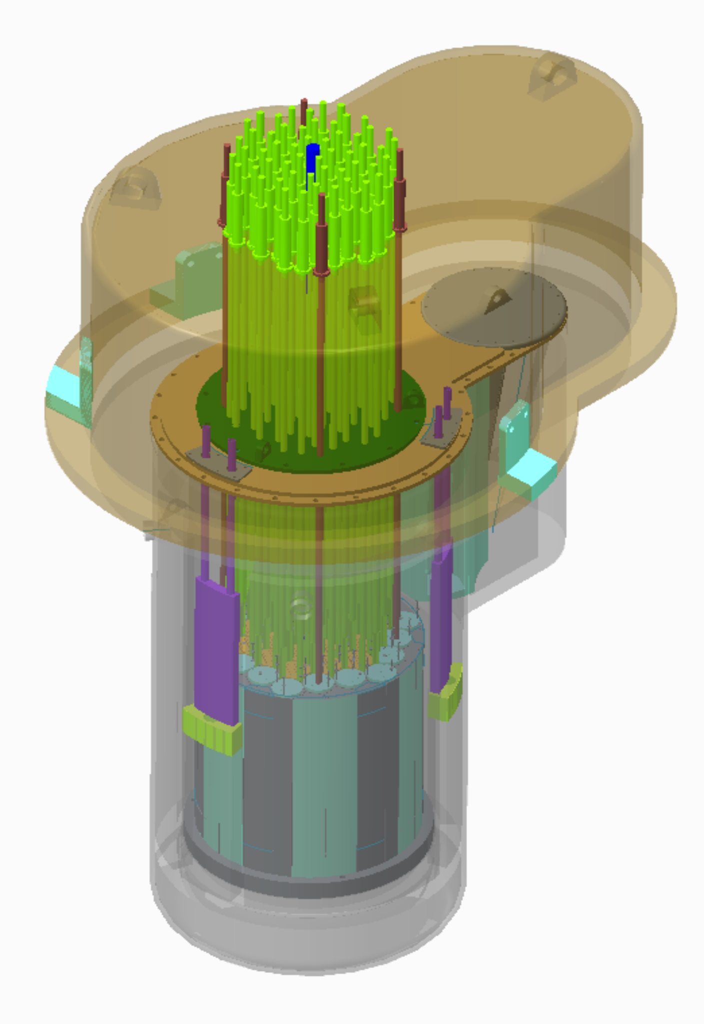
Molten Salt Reactor Experiment Benchmark Evaluation

(Max Fratoni, maxfratoni@berkeley.edu; Jeff Powers, powersjj@ornl.gov; Germina Ilas, ilasg@ornl.gov)

- An FY17-19 DOE NEUP award supports the development of a high-quality benchmark to benefit the MSR nuclear community.
- Effort is led by Max Fratoni, UC Berkeley, with collaborators from Oak Ridge National Laboratory and Grenoble Institute of Technology .
- Currently, the International Reactor Physics Benchmark Experiment Evaluation Project (IRPhEP) handbook does not contain any benchmark related to MSR technology - knowledge gap of high priority.
- The new IRPhEP benchmark will be based on the unique legacy data of the Molten Salt Reactor Experiment (MSRE), operated at ORNL from 1965 to 1969.
- Multiple M&S packages will be used in the study: SCALE, MCNP, NEAMS, Serpent, Monteburns.

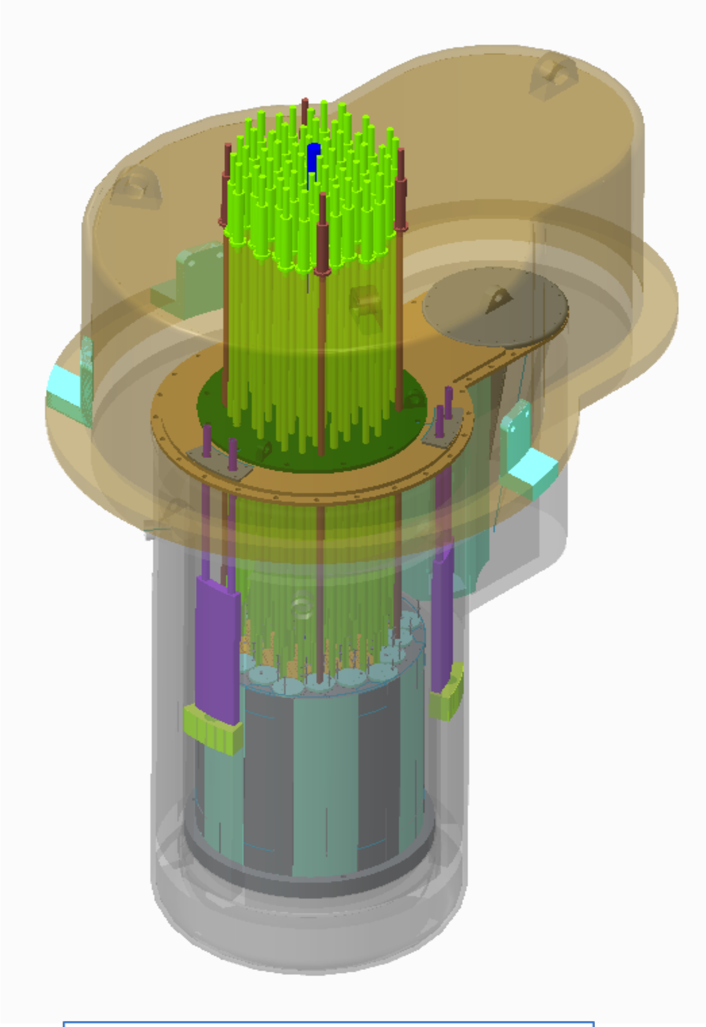


FHR-Demonstration Reactor Point Design

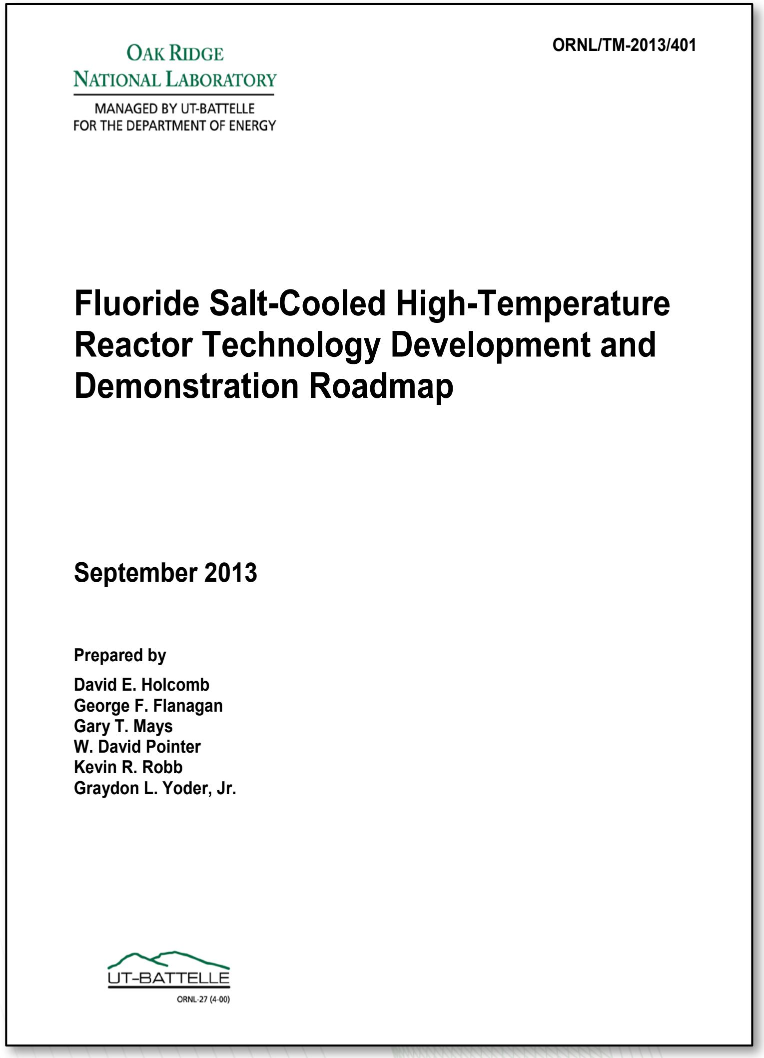


The ATDR FHR DR activity identified several needs
(Lou Qualls, quallsal@ornl.gov)

- Testing/qualification of fuel
- Structural material performance
- High temperature operation
- Passive safety system response
- M&O including fuel handling
- Pumping and heat exchange
- Tritium management
- Fission product lifecycle modeling
- Salt stability and activation
- Chemistry control



FHR Demonstration Reactor Point Design



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ORNL/TM-2013/401

Fluoride Salt-Cooled High-Temperature Reactor Technology Development and Demonstration Roadmap

September 2013

Prepared by
David E. Holcomb
George F. Flanagan
Gary T. Mays
W. David Pointer
Kevin R. Robb
Graydon L. Yoder, Jr.

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ORNL-27 (4-00)

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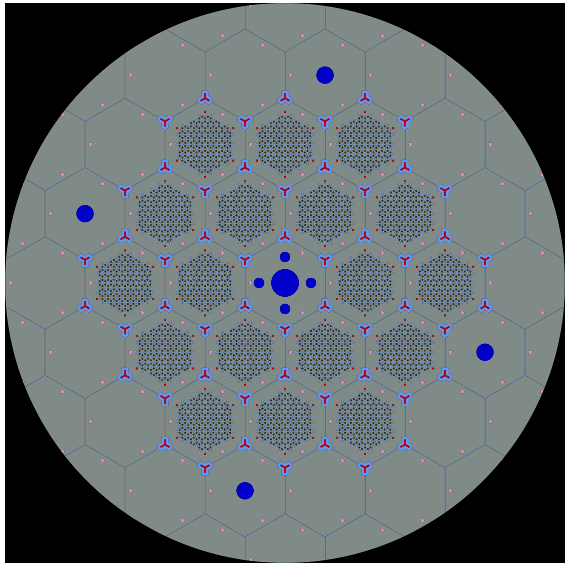
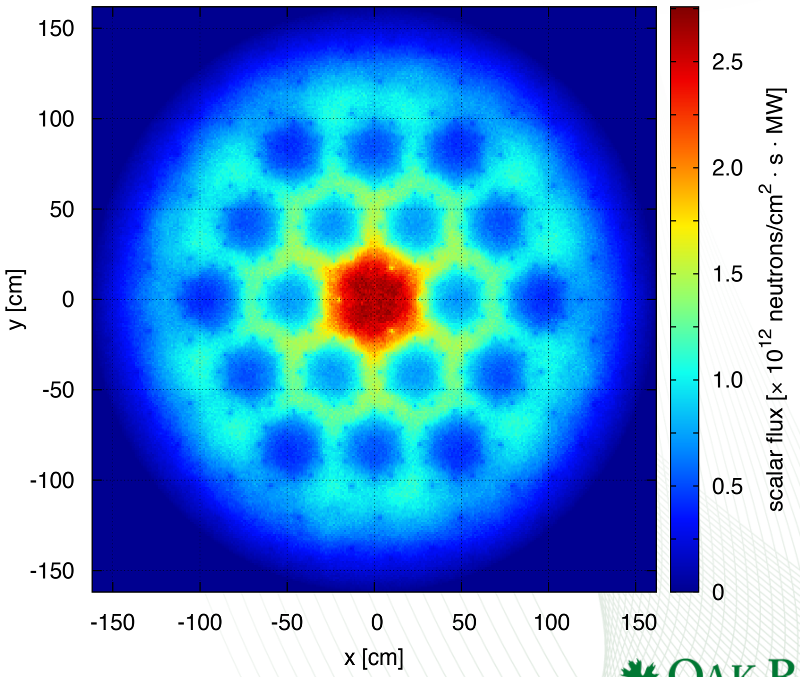
FHR DR Core Modeling Tools

(Aaron Wysocki, wysockiaj@ornl.gov)

- **Initial FHR DR Design**
  - Single batch core lifetime of 12 to 18 months
  - 100 MWt
  - Graphite block-type core
  - TRISO fuel with FLiBe coolant
- **Physics analysis tools: Serpent, PARCS, SCALE**
- **Thermal and systems analysis tools: RELAP5-3D, TRACE, COMSOL**
- **Availability**
  TRACE/PARCS: U.S. NRC
  SCALE: ORNL, rsicc.ornl.gov
  RELAP5-3D – INL, www4vip.inl.gov/relap5/
  Serpent – VTT, rsicc.ornl.gov
  COMSOL – comsol.com





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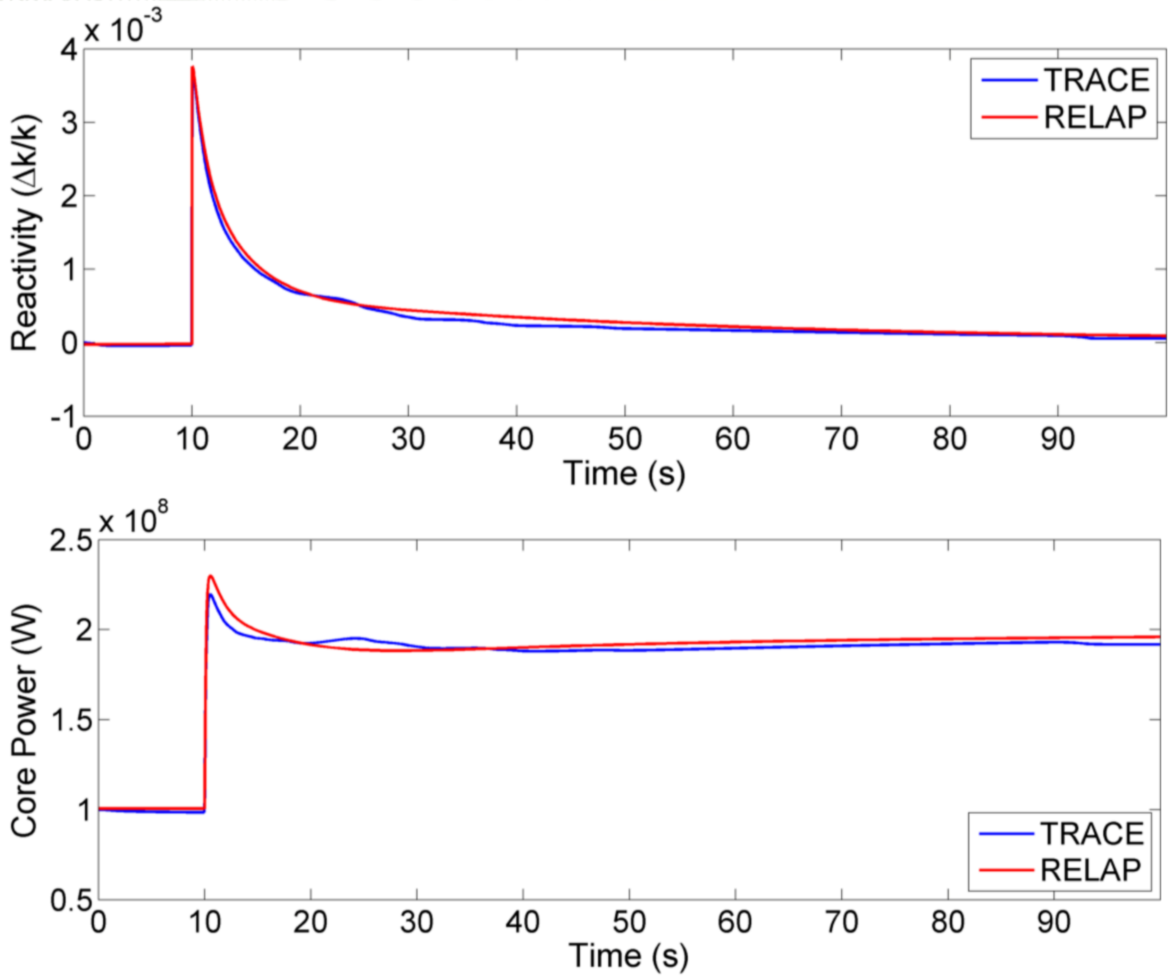
RELAP5-3D and TRACE Simulations for the FHR DR

(Aaron Wysocki, wysockiaj@ornl.gov)



- Rapid control rod withdrawal without SCRAM modeled using an instantaneous reactivity insertion
- Instantaneous reactivity insertion is not a credible scenario due to the lower pressure in the system, but provides limiting estimations of power, temperature, etc.
- Pumps remain at 100% flow through the transient
- Validated extensively for LWRs, limited validation data available for MSRs

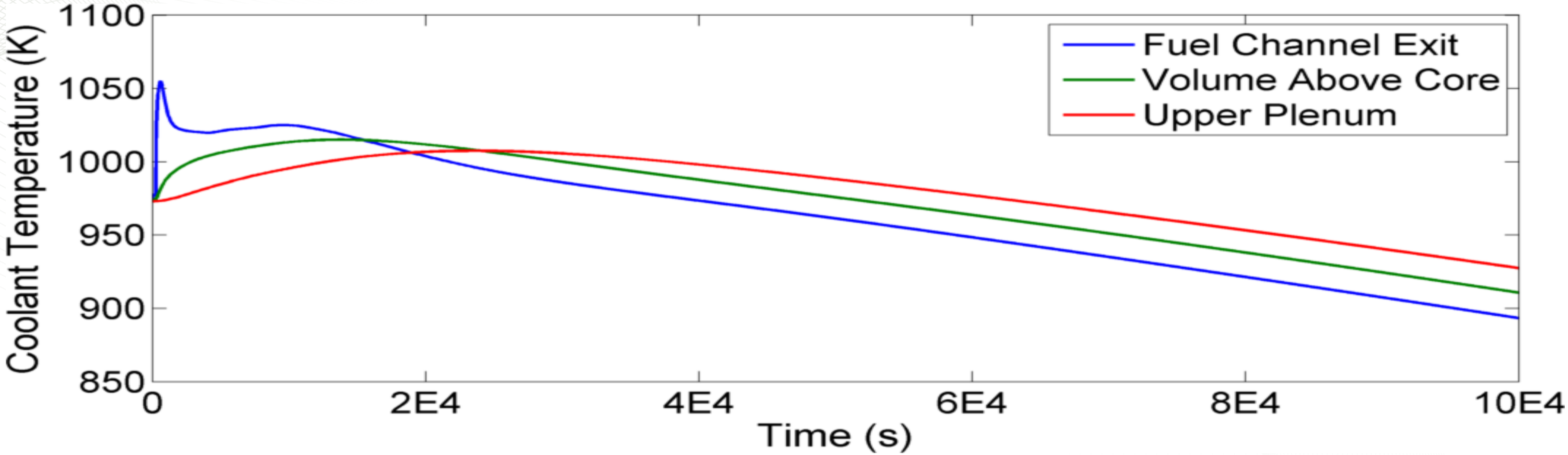
<u>Good agreement between RELAP5-3D and TRACE models using feedback effects</u>

Safety analysis considered for FHR-DR

- Anticipated Operational Occurrences (AOOs) and Design Basis Accidents (DBAs) were defined
  - increase or decrease in heat removal from the primary coolant,
  - decrease in reactor coolant system flow rate,
  - reactivity accidents,
  - increase or decrease in reactor coolant inventory,
  - radioactive release from a subsystem or component.

- FHR DR safety analysis emphasized the following transients:
  - LOFF with SCRAM,
  - LOFF without SCRAM,
  - Overcooling transients,
  - Reactivity initiated accidents.

Response after Loss of Forced Flow Accident



- LOFF with SCRAM
- One DRACS is assumed inoperable
  - one active and one passive DRACS modeled
- Preliminary analyses suggests coolant temperatures remain below limits for structural materials

Ongoing ORNL MSR M&S Activities

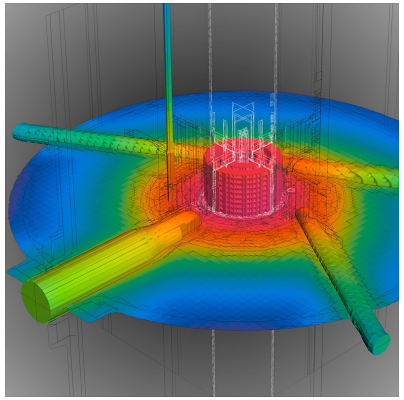
- General Neutronics
  - Multigroup library group structure for MSR and HTGR – Lukasz Koszuk (visiting PhD student)
  - Generation of MG cross sections using Shift in SCALE for NRC – Brian Ade, adebj@ornl.gov
  - Reference continuous energy depletion with Shift in SCALE for NRC – Brian Ade
  - Uncertainty quantification for advanced reactor neutronics in SCALE for NRC – Will Wieselquist, wieselquiswa@ornl.gov
- Molten Salt Fuel
  - ChemTRITON script for SCALE – Ben Betzler, betzlerbr@ornl.gov
  - Delayed neutron precursor drift capabilities in SCALE – Ben Betzler
  - Continuous feed and removal in TRITON – Ben Betzler
  - MSR Plant Dynamic Simulation with Delayed Neutron Precursor Drift – Scott Greenwood, greenwoodms@ornl.gov; Jordan Rader, raderjd@ornl.gov
- MSR Multiphysics
  - LDRD on development of a MSR core simulation capability – Ben Collins, collinsbs@ornl.gov

Shift and SCALE Integration

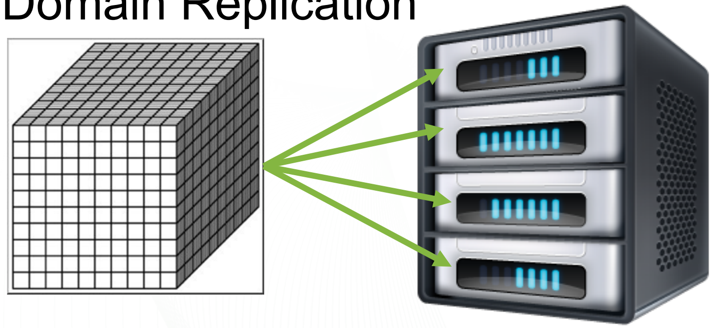
(Brian Ade, adebj@ornl.gov; Greg Davidson, davidsongg@ornl.gov)

- Shift – next generation Monte Carlo neutron transport code
  - Significant development to support advanced reactors such as HFIR
- Domain decomposed – will run on laptops through leadership-class clusters
- Currently being integrated into SCALE for criticality and for depletion analyses
- Uses TRITON's flexible interface for depletion analysis that allows time-dependent changes in multiple parameters
- Will be capable of generating broad-group data for nodal diffusion calculations from a continuous-energy solution
- Demonstration of the new capabilities using advanced reactor test problems (HTGR, MSR, etc.) with be documented by the end of 2017

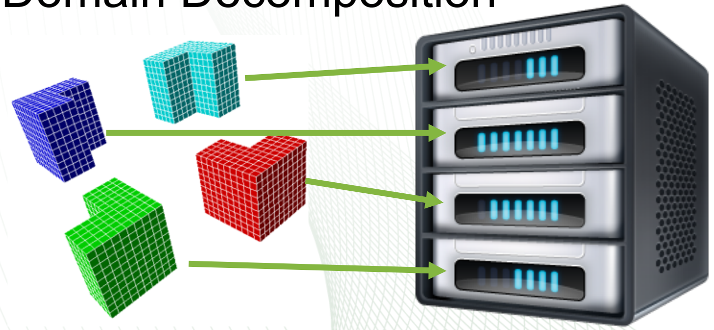
HFIR Flux



Domain Replication



Domain Decomposition



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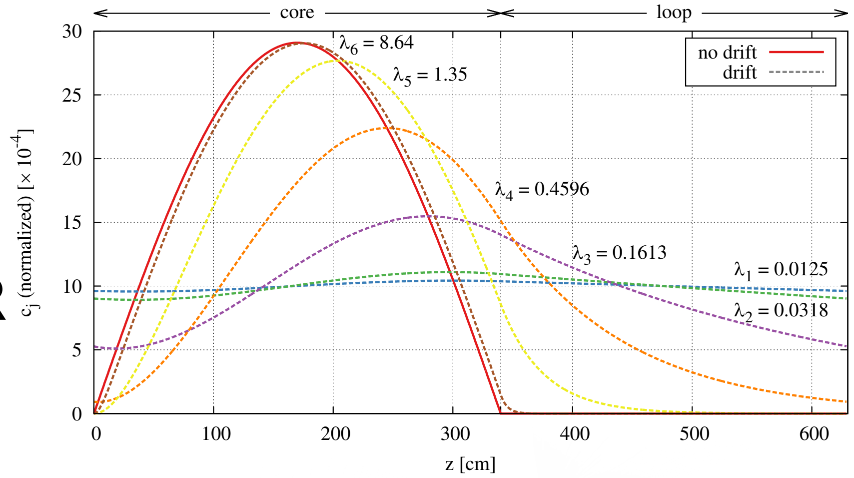
Core Neutronic Analysis for MSRs

- **Delayed neutron precursor drift in flowing fuel**
  - Delayed neutron precursors are radioactive fission products that release delayed neutrons upon decaying
  - In solid fuel systems, the movement of these delayed neutron precursors is negligible
  - In liquid fuel systems, the precursors move away from their birth location and may decay outside of the core, *changing the neutron source within the core*
- **Depletion with continuous and batch feeds and removals**
  - Continuous processes in liquid fuel systems remove fission gases and potentially other fission products during operation
  - Material may be added to and removed from the liquid in batches at discrete intervals
  - Serpent does have a continuous removal capability

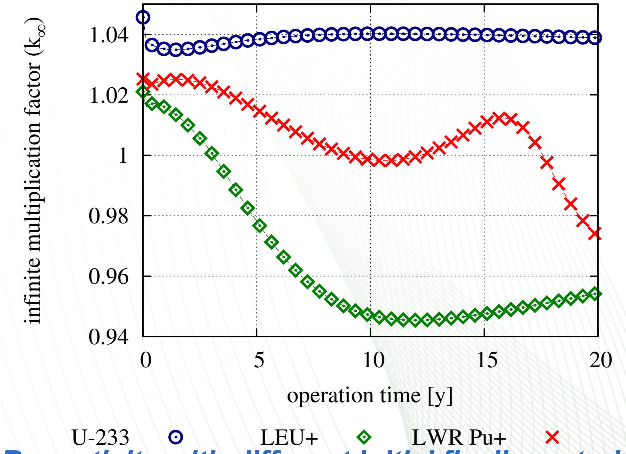
MSR-Specific Neutronic Modeling Improvements

(Ben Betzler, betzlerbr@ornl.gov)

- **Technology Commercialization Fund for MSR Tools Development**
  - Develop a software package capable of calculating MSR fuel composition and reactivity changes during operation
  - Develop delayed neutron precursor drift model within SCALE neutronics capability
  - Integrate chemical removal capability demonstrated by ChemTriton tool
- **ChemTriton internal script**
  - Models the changing isotopic composition of an irradiated fuel salt using SCALE for neutron transport and depletion calculations



Delayed neutron precursor concentrations in the primary loop of a liquid-fueled MSR.

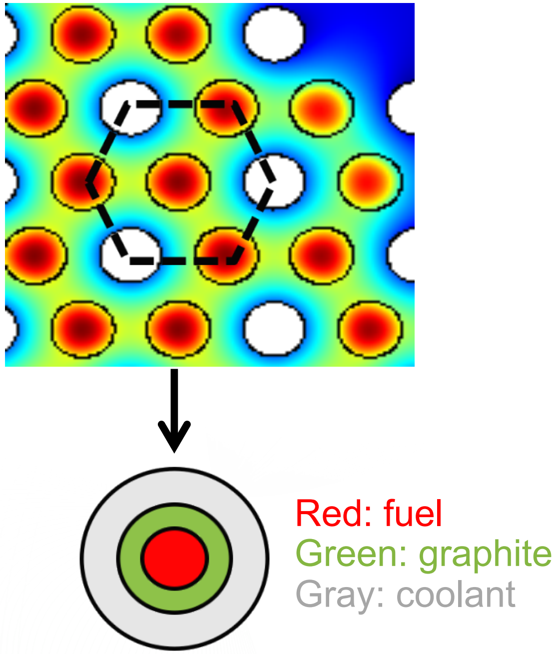


MSR reactivity with different initial fissile materials.

TRACE/PARCS MSR Capabilities

(Aaron Wysocki, wysockiaj@ornl.gov)

FHR prismatic design: conversion to "LWR-like" cylindrical fuel geometry



Description:

- U.S. NRC coupled 3D thermal hydraulic/neutron kinetic solver

Benefits:

- Performs assembly-level TH and neutronic calculations
- Allows modeling of full primary loop
- Runtime: less than 1 hour on single workstation

Capabilities Added for MSRs:

- Addition of molten salt fluid properties to TRACE (delivered to NRC in 2016)

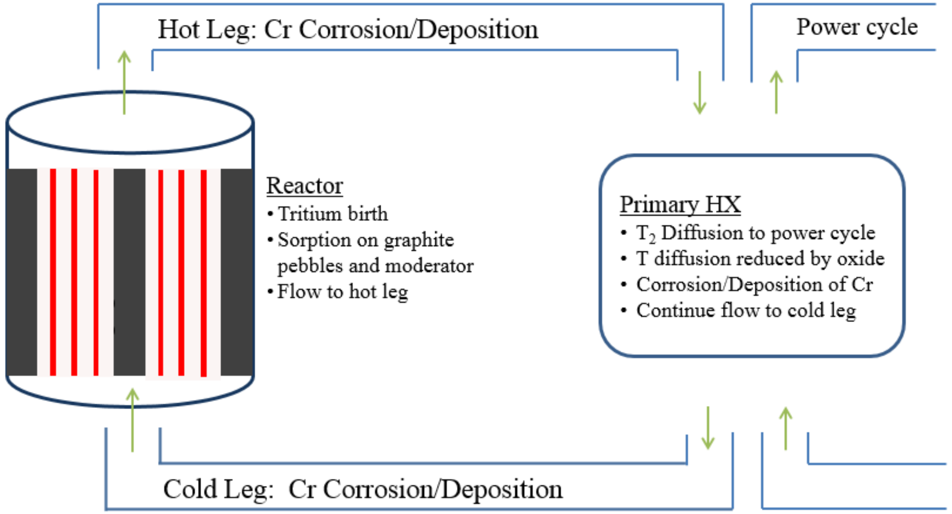
Challenges/Future Plans:

- *Salt-cooled designs*: special treatment needed to convert fuel geometries (e.g. FHR hexagonal lattice) to an equivalent "LWR-like" cylindrical fuel geometry approximation
- *Salt-fueled designs*: Capability must be added to track precursor transport in molten salt primary loop, to capture steady-state and transient reactivity effects

TRIDENT TRITium Diffusion EvolutioN and Transport

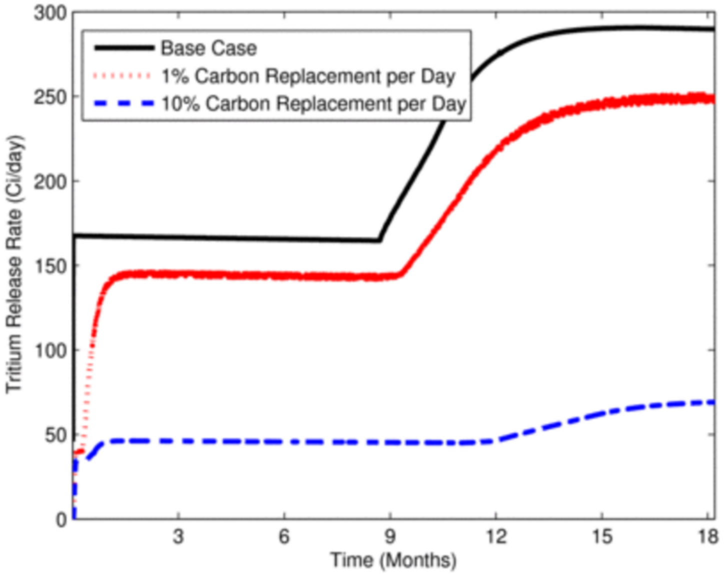
(Scott Greenwood, greenwoodms@ornl.gov)

- 2015 Doctoral research project of John Stempien (MIT)
- Objective:
  - Predict tritium distribution and release rates in FHR systems (primary and secondary loops)
  - Account for different behavior of TF and T2
  - Evaluate effectiveness of tritium capture systems
  - Account for coupling between corrosion and tritium behavior
  - Predict corrosion rates



A representation of the loops evaluated in TRIDENT and the kind of physics included in the model

- Modifications:
  - Original TRIDENT programmed for pebble bed type reactor
  - Modified input files were generated to better reflect the reactor core geometries of the FHR-DR
  - Tritium production rates modified
- Recommendations:
  - The current version of TRIDENT represents a first attempt at providing a flexible tool to evaluate tritium issues.
  - ***Additional effort should be made to create a more general tool which would be more accurate, faster and more user-friendly***



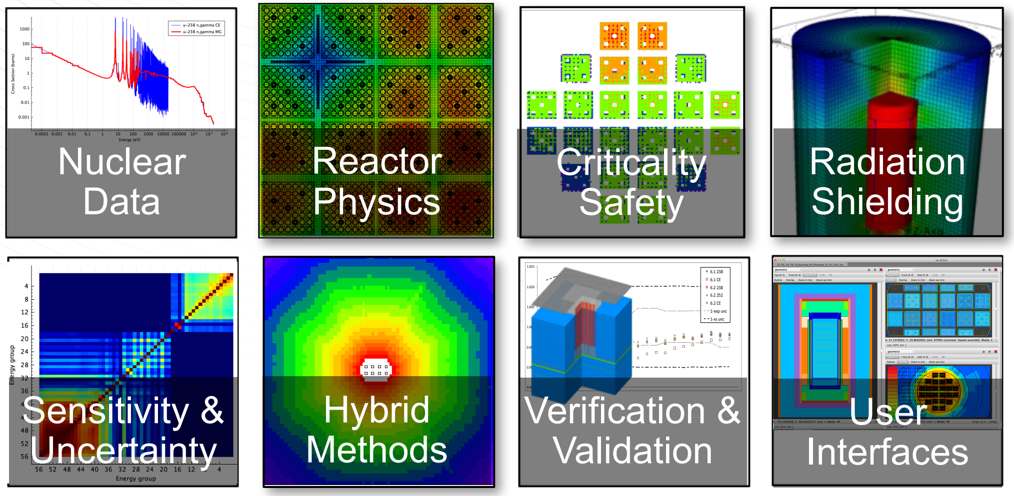
FHR-DR Tritium Production and Release Modeling using TRIDENT

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

SCALE Code System

Neutronics and Shielding Analysis Enabling Nuclear Technology Advancements
http://scale.ornl.gov

Practical Tools Relied Upon for Operations and Regulation



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FY16 Statistics:

- **12 week-long courses**
- **1 conference tutorial**
- **150 participants from 15 nations**

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NNSA National Nuclear Security Administration
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Tritium Production in SCALE

(Matthew Jessee, jesseema@ornl.gov)

- Tritium is safety concern for some MSRs because lithium-activation produces orders of magnitude higher amounts of tritium than LWRs
- Tritium production physics have been improved in SCALE 6.2
- Validated with MSRE benchmark data: R. B. Briggs, “Tritium in Molten-Salt Reactors,” *Reactor Technology*, **14(4)**:335 (Winter 1971-1972)

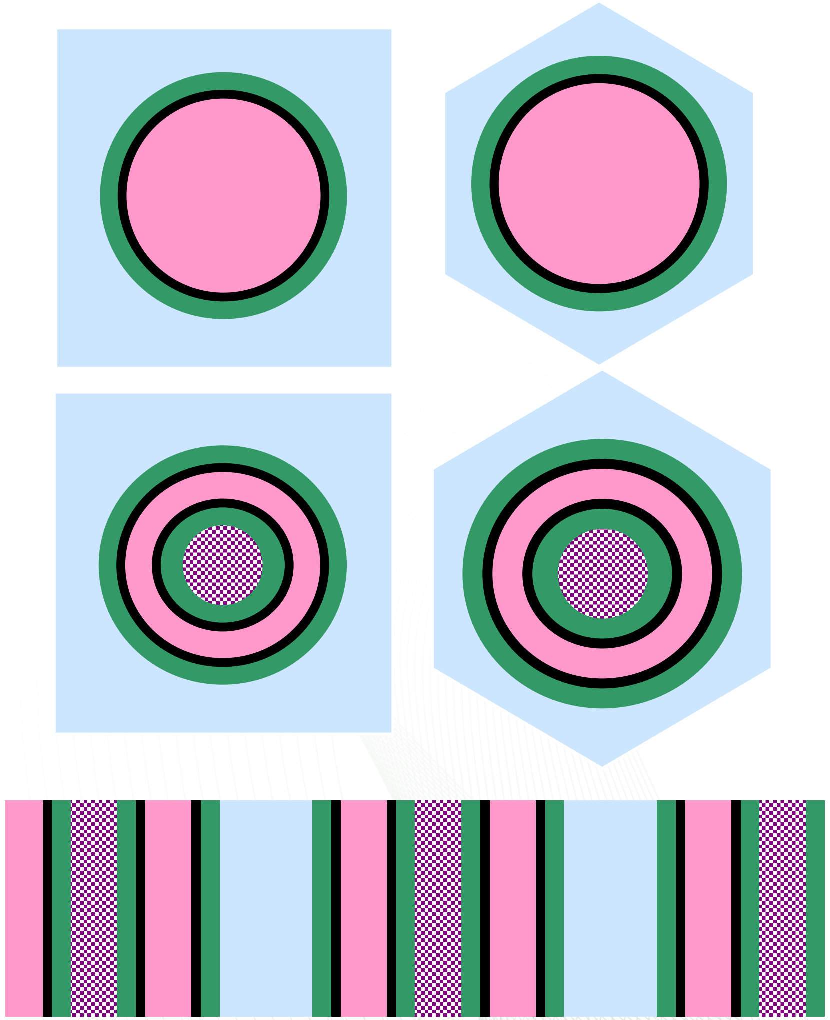
Nuclide	Measured (Ci/MTU)	SCALE 6.2 (Ci/MTU)	C/E
H-3	8.12E+04	1.11E+05	1.37

Note that the SCALE results above were based constant irradiation of 375 days with specific power of 30 MW/MTU to simulate the tritium production of ORNL MSRE. Enrichment of Li-7 is 99.99%. <u>SCALE 6.2 results agree within precision of experimental measurement.</u>

Double Het. Modeling Capability Expanded in SCALE 6.2

(Matthew Jessee, jesseema@ornl.gov)

- Cross-section processing methods for particle-based fuel (TRISO) have been available since SCALE 6.1.
  - Cylinders in square- or triangular-pitched arrays
  - Spheres in square- or triangular-pitched arrays
- New capabilities available in SCALE 6.2
  - Slab or plate fuel
  - Annular cylinders in square- or triangular-pitched arrays
  - Annular spheres in square- or triangular-pitched arrays



Multiphysics Core Simulation of MSRs

(Ben Collins, collinsbs@ornl.gov)

Description:

- ORNL LDRD which leverages CASL-driven high fidelity core simulator capability and extends to MSRs using MPACT/CTF

Benefits:

- High-fidelity (sub-channel, sub-fuel-pin) coupled TH/neutronic calculations
- Runtime: Industry class compute cluster <u>(100-1000 cores) and ~30 minutes per statepoint</u>

Capabilities Added for MSRs by ORNL LDRD:

- Addition of molten salt fluid properties to CTF
- Model for continuous feed and removal of material in primary loop.
- Precursor transport in molten salt primary loop, to capture steady-state reactivity effects

Ongoing Work:

- Extension of geometry and heat conduction solver for rectangular and hexagonal geometries
- Modeling the bulk formation of chemical species via chemical and nuclear reactions

MPACT/COBRA-TF Coupled Physics

(Ben Collins, collinsbs@ornl.gov)

MPACT
(Reactor Physics)

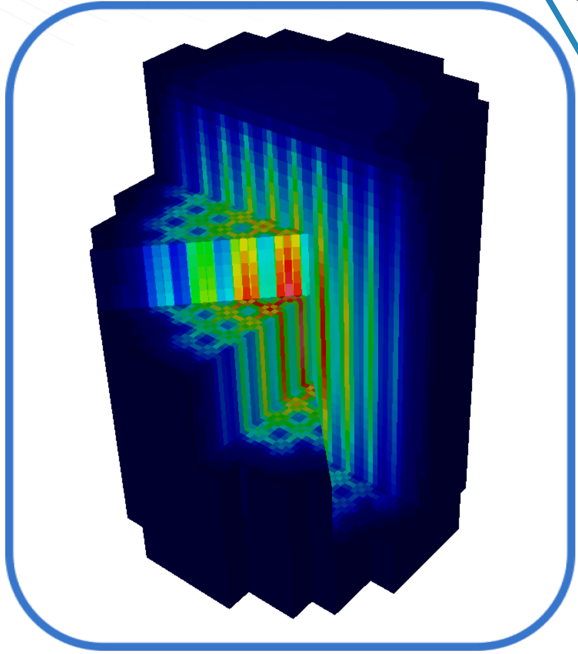
Power Generation Rate

CTF
(Thermal Hydraulics)

Temperature and
Coolant Flow and Density

Isotopic Generation Rate

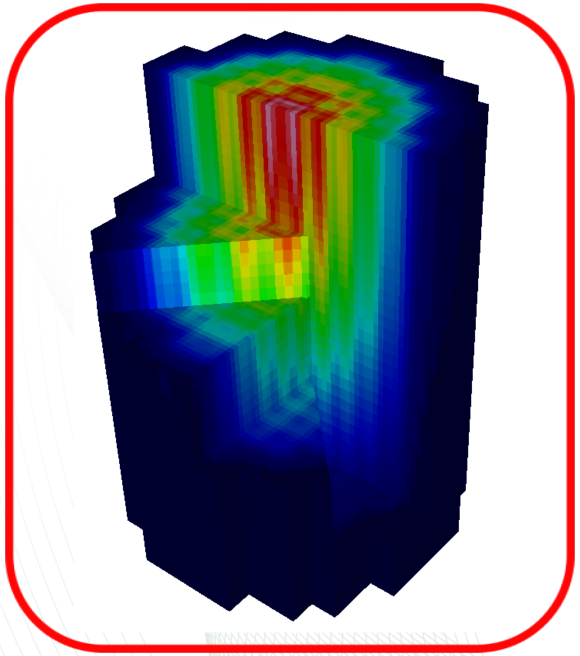
Isotopic Distribution



- **Homogeneous Speciation:** models for the bulk formation of chemical species via chemical reactions and nuclear reactions (reaction sources)
- **Bulk Transport:** convection and diffusion of multi-species (thermodynamic and transport properties)
- **Interfacial Transport:** liquid-solid interfaces (corrosion), liquid-gas interface (off-gas)
- Continuous fuel processing (addition/removal)

Multi-species
Mass Transport

Coolant Flow and
Temperature Distribution



Gap Analysis – Where and when can we help?

- Solid Fuel Neutronics
  - **Shift:** CE and MG Monte Carlo-based depletion + XS generation. → available in SCALE 6.3
  - **TRITON:** CE and MG multigroup depletion (Monte Carlo and Deterministic) + XS generation. → available now in SCALE 6.2
- Salt Fuel Neutronics
  - **ChemTRITON:** Currently an ORNL internal script. These capabilities are being added to TRITON (2D) to model precursor drift and continuous feed/removal. → available in SCALE 6.3
- Coupled Neutronics & TH
  - **TRACE/PARCS**: Systems TH analysis + kinetics provided by nodal diffusion. Salt properties recently added. → Contact U.S. NRC for availability
  - **MPACT/CTF:** Highly detailed multiphysics simulations. Hex geometry, precursor drift, salt TH, being added under LDRD. → Fall 2018, availability to be determined

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Gap Analysis – Where and when can we help?

- Plant Dynamics
  - **TRANSFORM:** Toolkit for plant dynamics and systems modeling for MSRs using Modelica. → ORNL internal code
- Tritium Transport
  - **TRIDENT:** Prediction of tritium distribution and release rates in FHR systems. → ORNL internal code
- Data
  - **MSRE Benchmark**: Funded under NEUP for FY17-19, UC-Berkley led with ORNL collaborators. → IRPhEP, 2019

MSR M&S Summary

- Several tools are available and/or under development to address MSR evaluation needs
  - Neutronic and thermal hydraulic performance
  - Dynamic system models
- Traditional models can be developed with adequate data
  - Chemistry and corrosion modeling
  - Materials response modeling
  - Passive safety system response
- New simulation capabilities are currently under development
  - Engagement of stakeholders, users, and developers is necessary to ensure needed capabilities are developed

SCALE Enhancements for Advanced Reactor Analysis

Brad Rearden (ORNL)

SCALE Enhancements for Advanced Reactor Analysis

Presented to:

Workshop on Tools for Modeling and Simulation of Fluoride Cooled High Temperature Reactors (FHR)

Georgia Institute of Technology
February 8-9, 2017

Bradley T. Rearden, PhD

Leader, Modeling and Simulation Integration
Manager, SCALE Code System
Leader, NEAMS Integration Product Line

ORNL is managed by UT-Battelle
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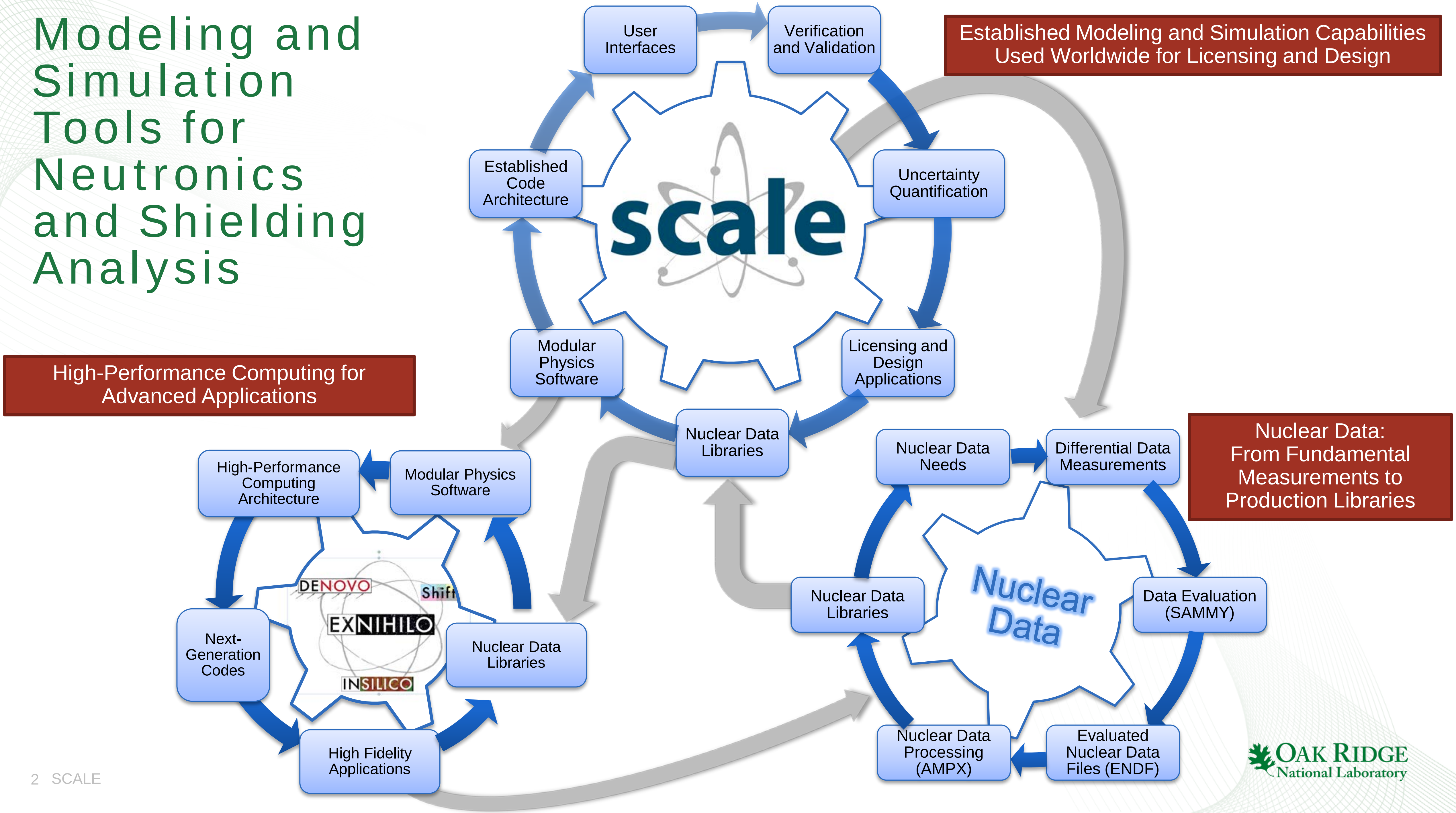
Modeling and Simulation Tools for Neutronics and Shielding Analysis



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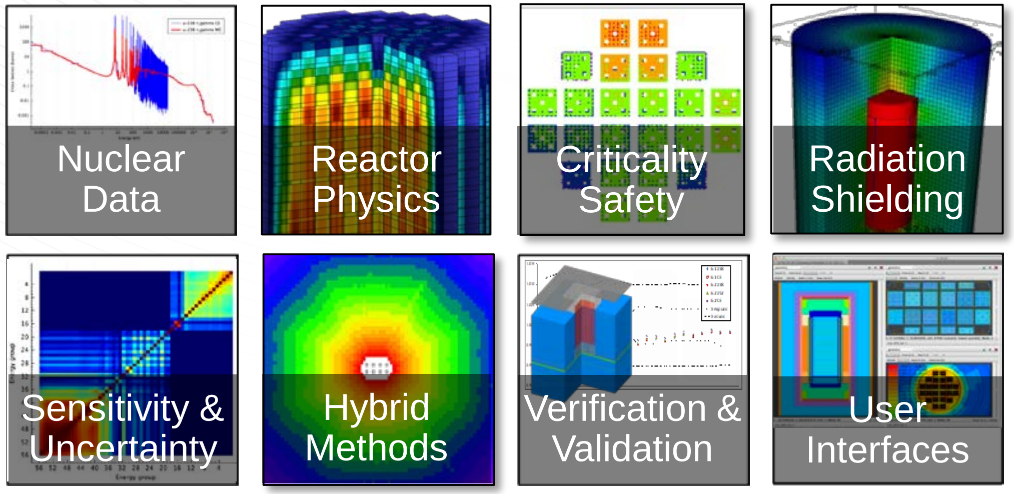

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SCALE 6.2 – April 2016

Innovative

- Modernized architecture for efficiency and quality
- Enhanced sensitivity and uncertainty analysis
- Problem-dependent temperature treatments for continuous-energy Monte Carlo
- Reference continuous-energy depletion

Efficient

- Accelerated lattice physics capabilities
- Reduced memory requirements
- Parallel calculations
- Rapid radioactive source term generation

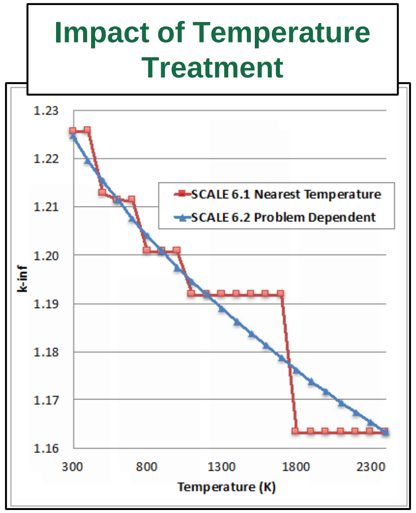
Accurate

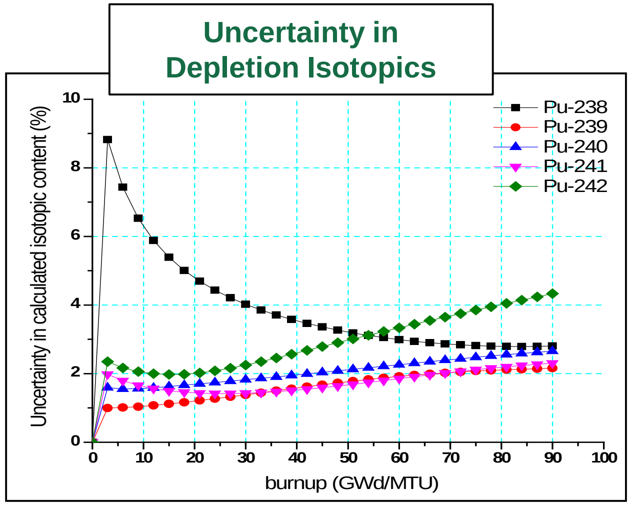
- Code and data enhancements to minimize historical biases
- Greatly expanded test suites for validation and verification

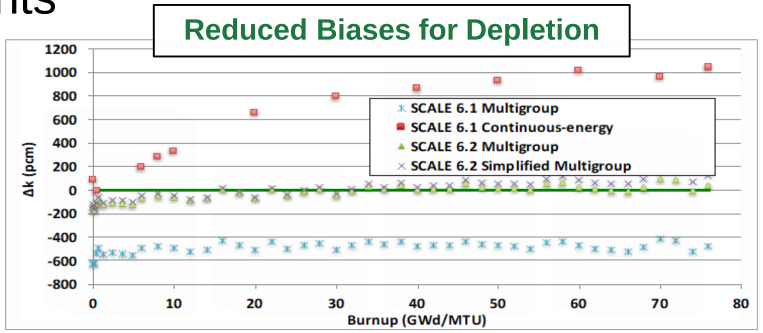
Easy to Use

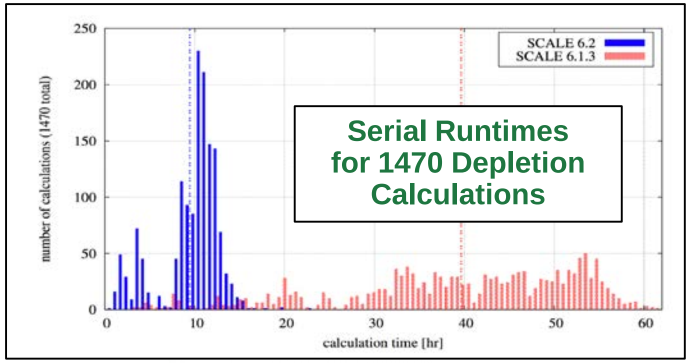
- Integrated user interface
- Simplified input

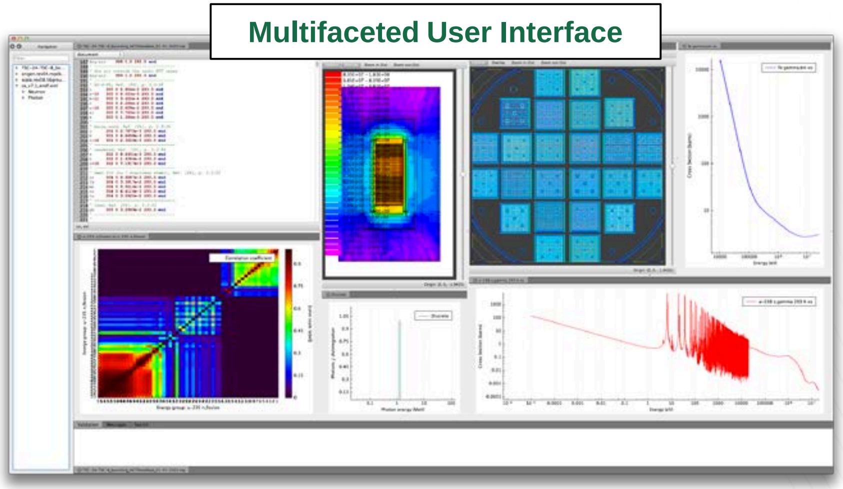
1700 licenses issued through January 2017

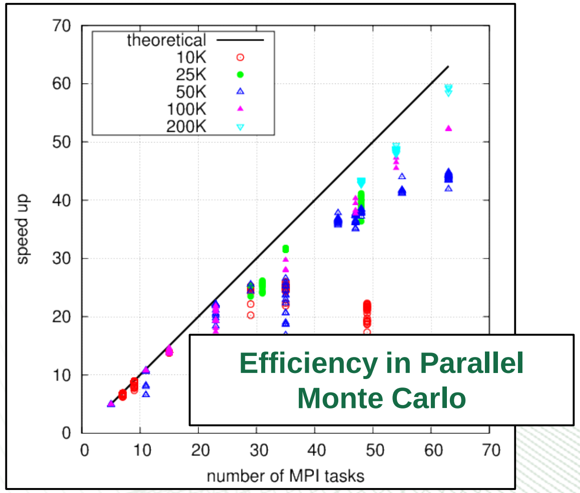








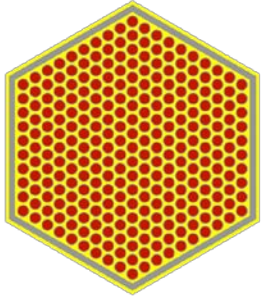




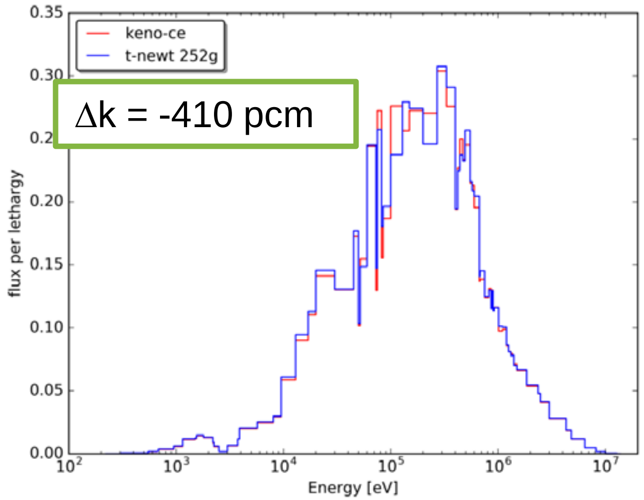
SCALE 6.2 Team Photo – May 2016

Left to right: Ahmed Ibrahim, Germina Ilas, Brandon Langley, Andrew Holcomb, Shane Hart, Cihangir Celik, Seth Johnson, Matt Jessee, Kevin Clarno, Adam Thompson, Bob Grove, Rob Lefebvre, Greg Davidson, Charles Daily, Alan Icenhour, Barbara Snow, Brian Ade, Brad Rearden, Ben Betzler, B. J. Marshall, Kursat Bekar, Will Wieselquist, Mark Baird, Mark Williams, Georgeta Radulescu, Ron Ellis, Thomas Miller, Dan Ilas, Elizabeth Jones, Cecil Parks, Sheila Walker, Teresa Moore, Marsha Henley, Sandra Poarch, Lester Petrie

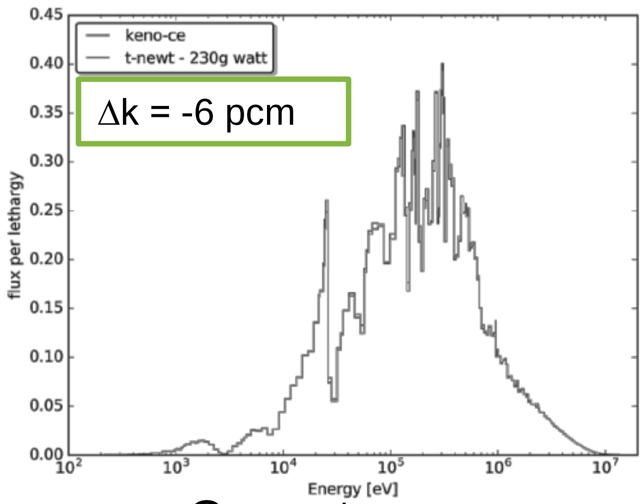
AMPX nuclear data processing tools deployed with SCALE



- Continuous-energy data serve as reference solution to confirm multigroup approximations
- SCALE 6.2 includes multigroup neutronics libraries that are optimized for LWRs
- Multigroup cross sections can be generated for any type of system
  – LWR, HTGR, MSR, FHR, SFR, etc. with appropriate energy group structure and weighting spectrum
- Uncertainties in cross sections (covariance data) quantify confidence in deployed data libraries
- Example for SFR:



Incorrect group structure/weighting



Correct group structure/weighting

Uncertainty in k_{eff} Due to Nuclear Data Uncertainties: 1,435 pcm!

covariance matrix				
nuclide-reaction		**with**	**nuclide-reaction**	**% Δk/k due to this matrix**
u-238	n,n'	u-238	n,n'	1.2053(9)
na-23	elastic	na-23	elastic	0.3242(2)
fe-56	elastic	fe-56	elastic	0.2590(3)
u-238	n,gamma	u-238	n,gamma	0.2435(1)
fe-56	n,n'	fe-56	n,n'	0.2388(1)

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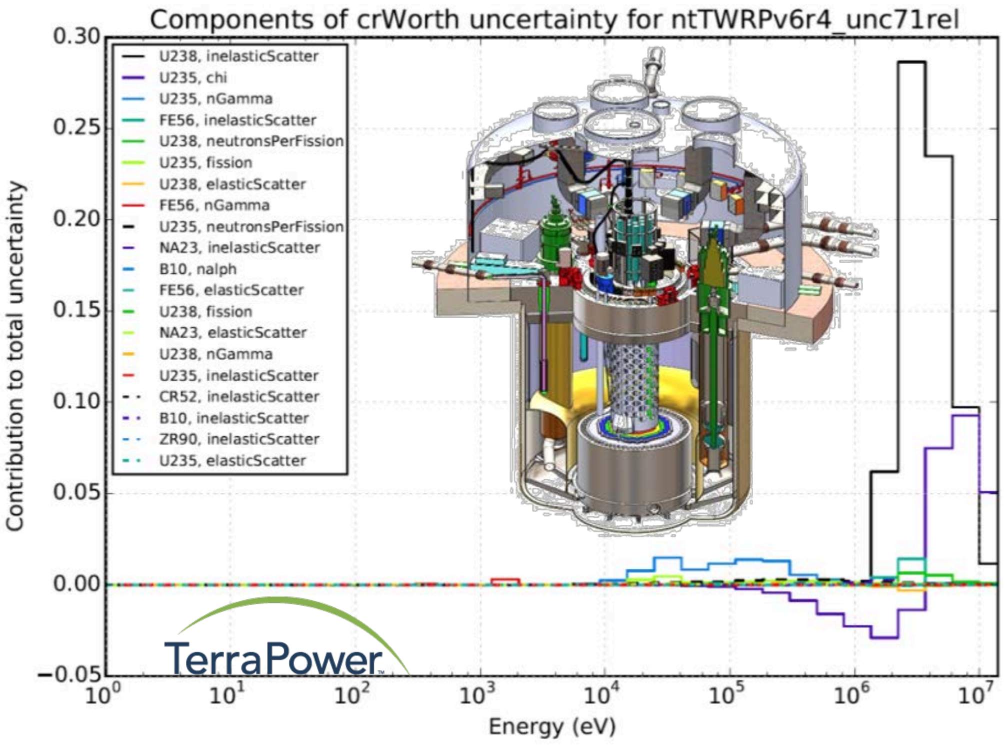
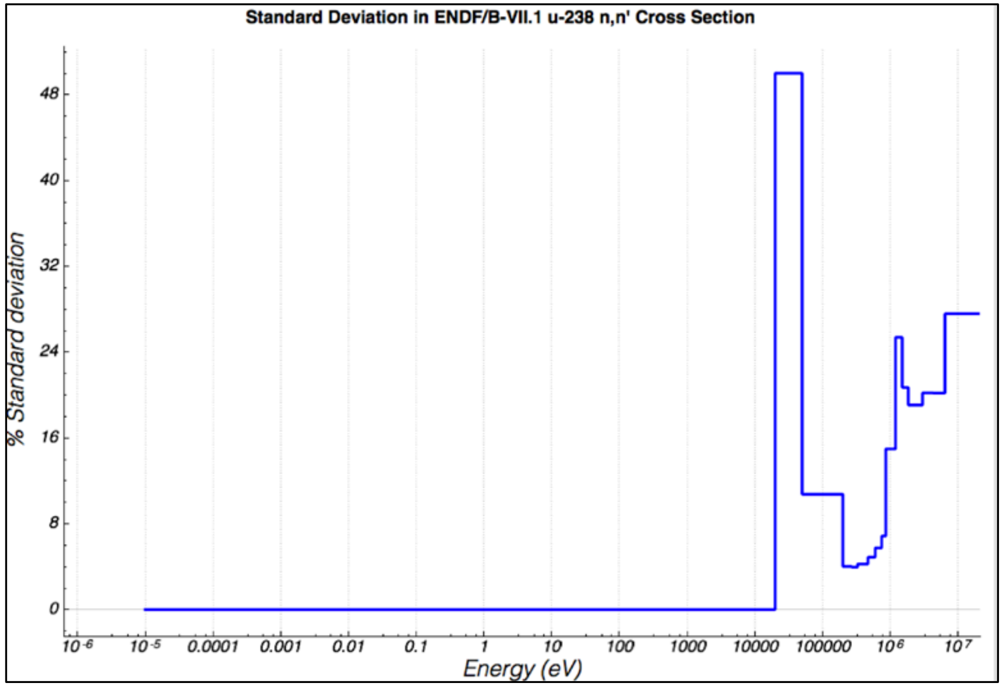
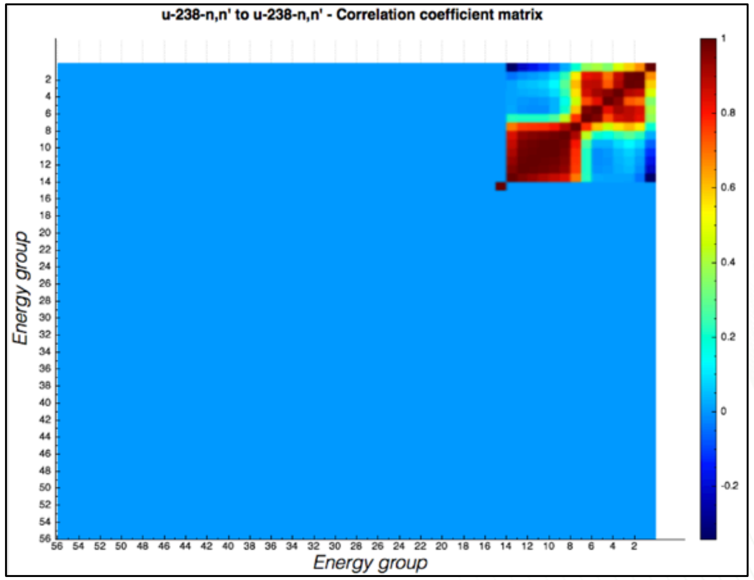
Nuclear Data Uncertainties

- Uncertainties in nuclear data can be a limiting factor in the design of advanced reactors
- ~3% uncertainty on control rod worth for TerraPower Traveling Wave Reactor



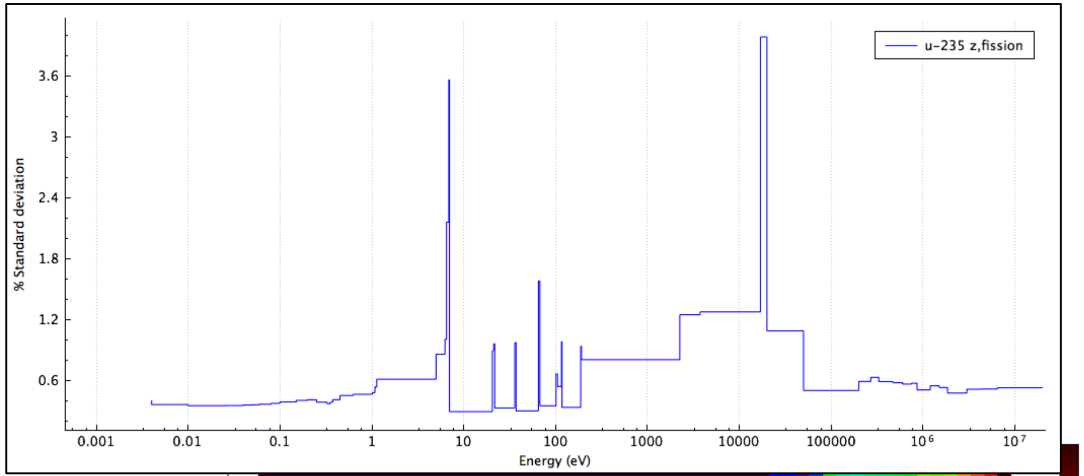


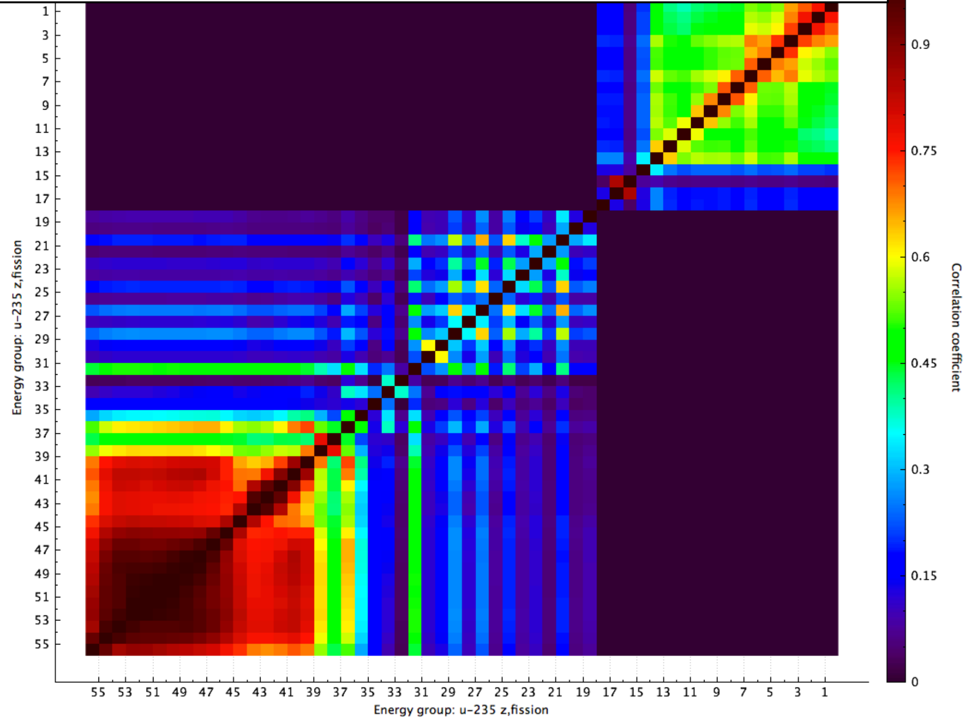


From: N. Touran, "Sensitivities and Uncertainties due to Nuclear Data in a Traveling Wave Reactor", NEA/OECD SG 39 Meeting 2016-05-10

SCALE 6.2 Covariance Library

- ENDF/B-VII.1 for 187 isotopes
- Modified ENDF/B-VII.1 ^{239}Pu nubar, ^{235}U nubar, H capture, and several fission product uncertainties, with data contributed back to ENDF repository for ENDF/B-VIII
- "Low-fidelity" data for ~215 nuclides missing from ENDF/B-VII.1
- Fission spectrum (chi) uncertainties processed from ENDF/B-VII.1 and from JENDL 4.0 (minor actinides)
  – Previous SCALE chi uncertainties were generated from Watt spectrum data and data were missing for minor actinides
- 56- and 252-group energy structures
- 33-group fast reactor library in development

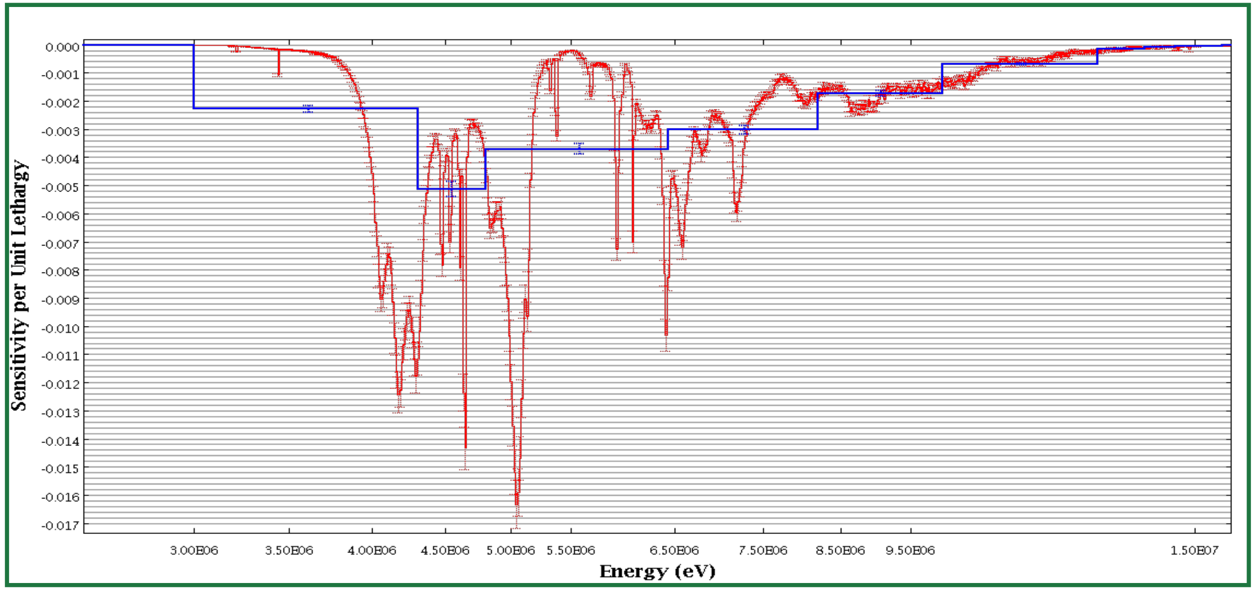




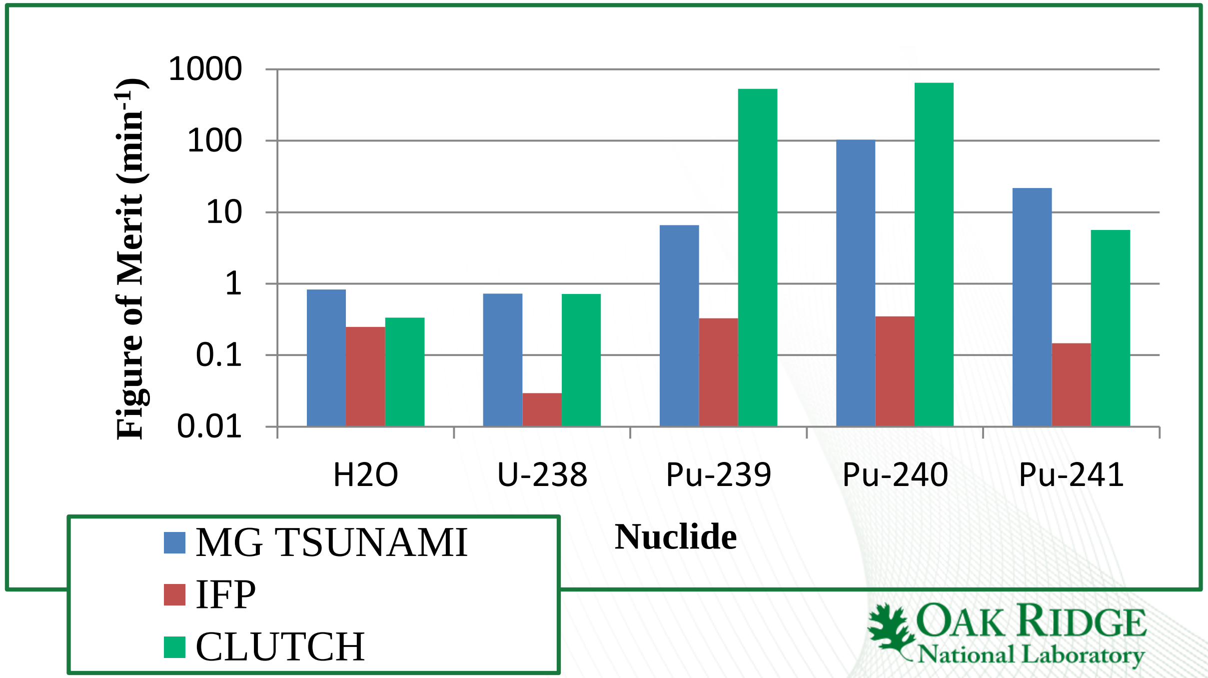
Continuous-energy TSUNAMI-3D

- In SCALE6.2 the multigroup TSUNAMI-3D code has been extended to perform continuous-energy (CE) sensitivity coefficient calculations.
  - ➢ This work involved the development of the CLUTCH sensitivity method, a new and efficient approach for calculating eigenvalue sensitivity coefficients.

O-16 Capture Sensitivity
238-group VS
Microgroup CLUTCH



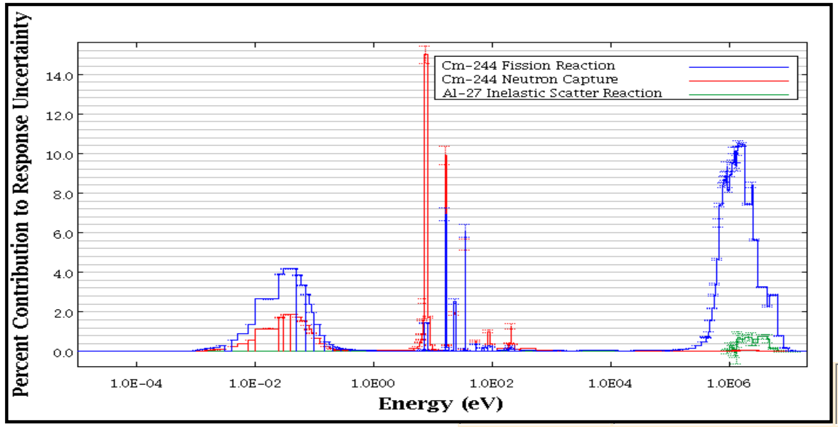
MIX-COMP-THERM-004-001
FoM Comparison

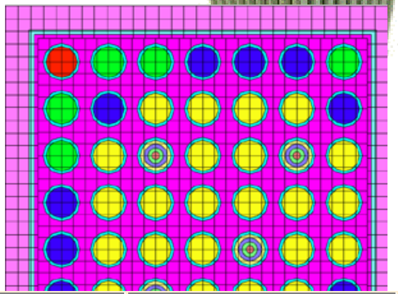


Generalized Perturbation Theory

- Recent developments have enabled the calculation of generalized response sensitivity coefficients using high-fidelity, continuous-energy Monte Carlo methods.

- Applications for GPT sensitivity/uncertainty analysis include:
  - Relative powers
  - Isotope Conversion Ratios
  - Multigroup Cross Sections
  - Experimental Parameters





Reaction Contributions to the Uncertainty in the ^{244}Cm Conversion Ratio	
^{244}Cm Fission Reaction	17.62%
^{244}Cm Neutron Capture	4.96%
^{27}Al Inelastic Scatter Reaction	0.72%
^{244}Cm Elastic Scatter Reaction	0.59%
^{1}H Elastic Scatter Reaction	0.56%
Total Data-Induced Uncertainty	**18.33%**

		Type	Format	Value	Xsec Uncert
1	k_infinity	keff	Relative	1.1083E+0	4.98551E-1 % dk/k
2	fission_grp_1	gpt	Relative	1.9155E-3	6.91925E-1 % dR/R
3	fission_grp_2	gpt	Relative	2.7748E-2	3.23440E-1 % dR/R
4	absorpt_grp_1	gpt	Relative	7.1637E-3	8.36728E-1 % dR/R
5	absorpt_grp_2	gpt	Relative	5.3702E-2	2.38082E-1 % dR/R
6	cornerrod_fpf	gpt	Relative	1.1458E+0	1.67147E-1 % dR/R

OECD UAM GPT Benchmark Phase 1-2 Results

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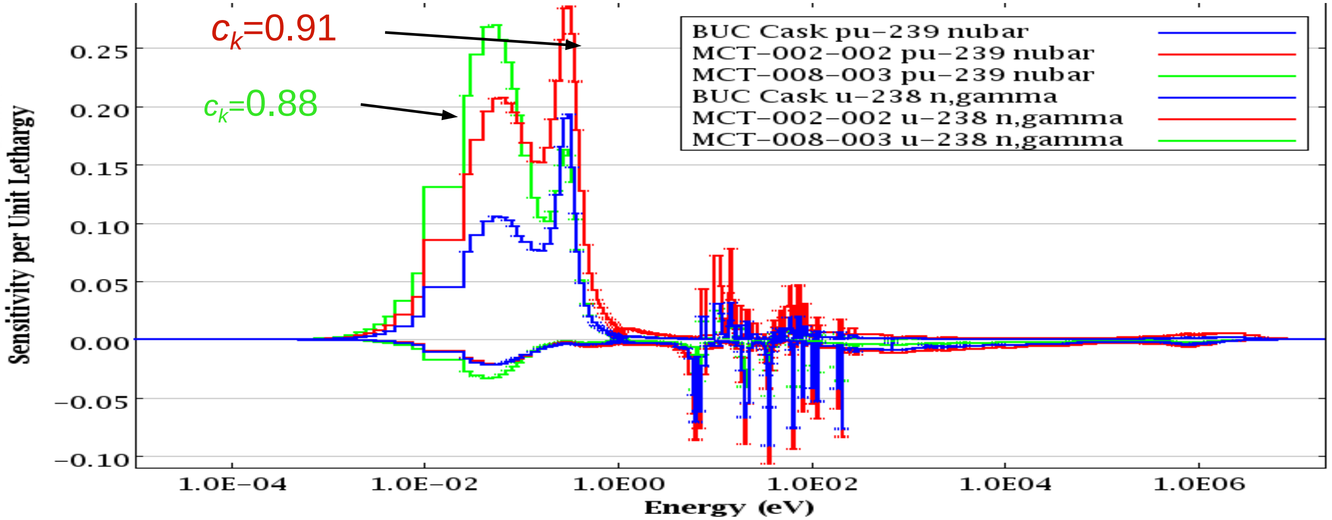
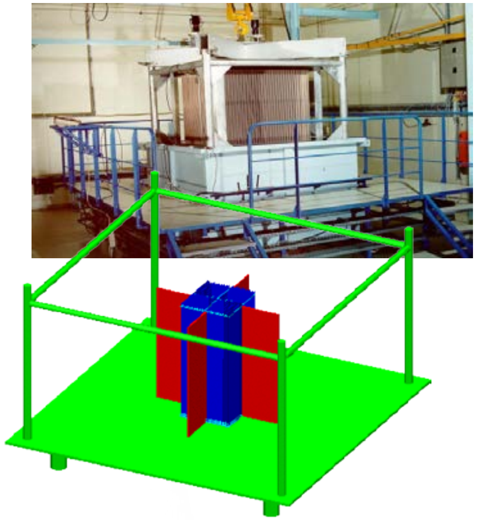
Advanced validation with sensitivity/uncertainty: Identifying experiments representative of targeted application

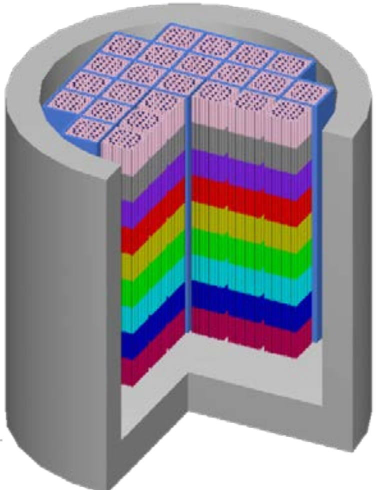
$$c_k^{(m,n)} = \frac{\mathbf{S}_{k_m}^{\mathrm{T}} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{k_n}}{\sqrt{Var(k_m)Var(k_n)}}$$

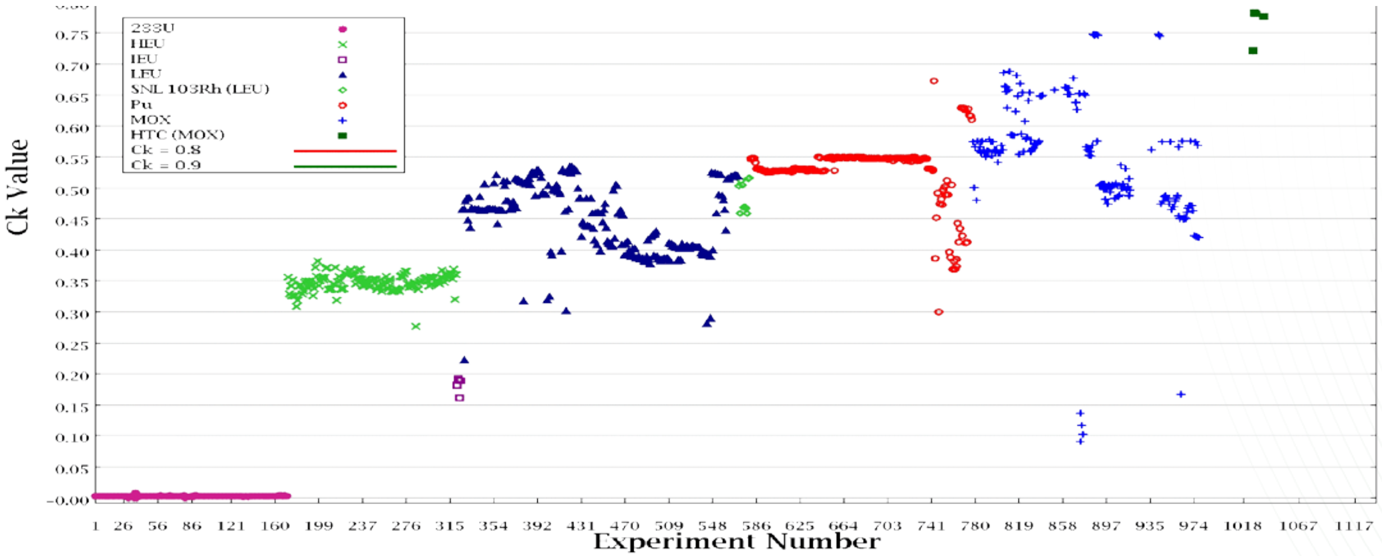


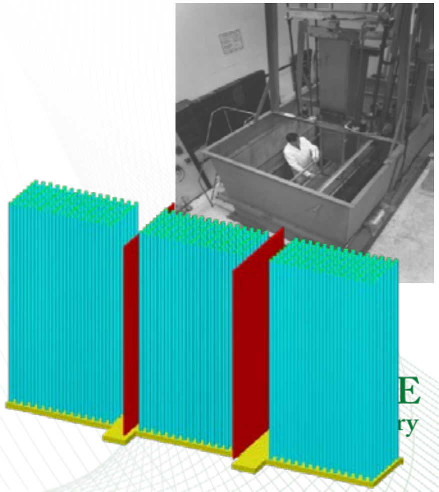


NUCLEAR CRITICALITY EXPERIMENTS

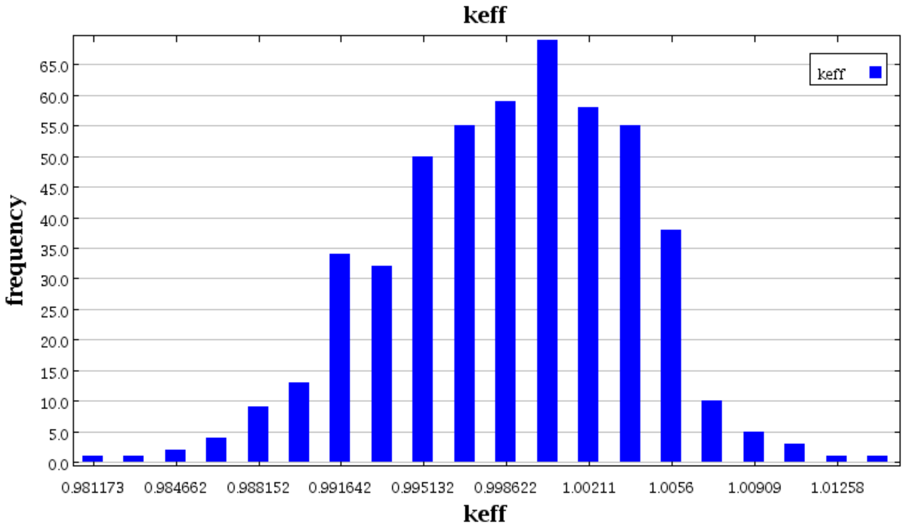
APPLICATION



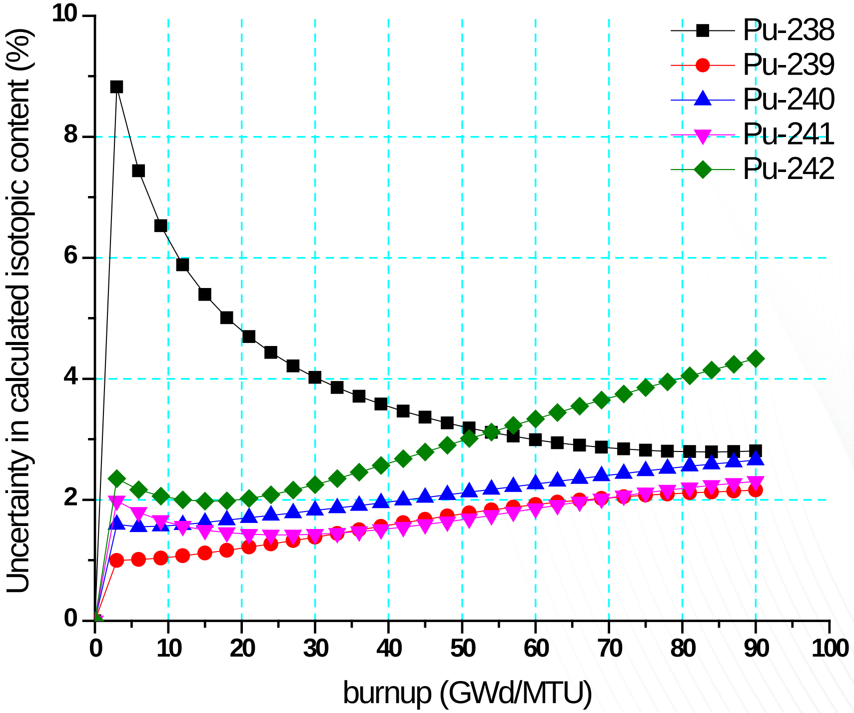




Sampler: A Module for Statistical Uncertainty Analysis with SCALE Sequences



- Sampler provides uncertainty in any computed result from any SCALE sequence due to uncertainties in:
  - neutron cross sections
  - fission yield and decay data
  - geometry and composition
- Sampler propagates uncertainties through complex analysis sequences such depletion calculations
- Correlations between systems are also computed



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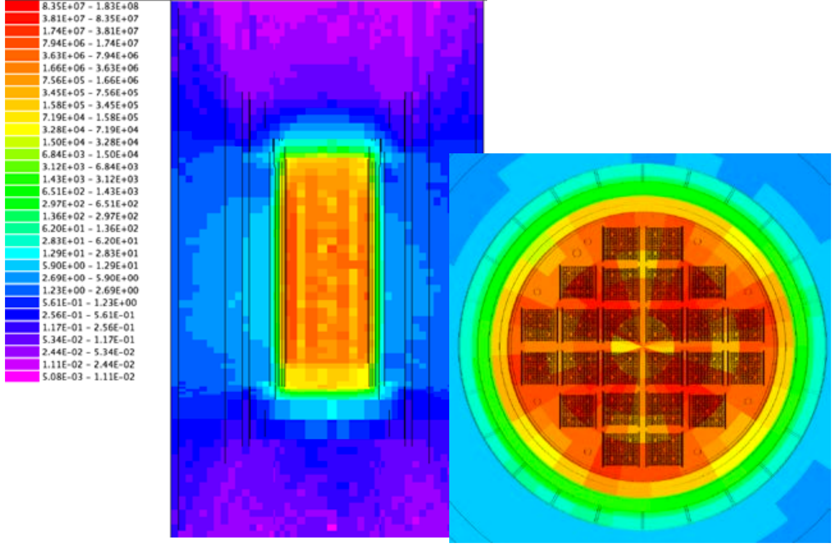
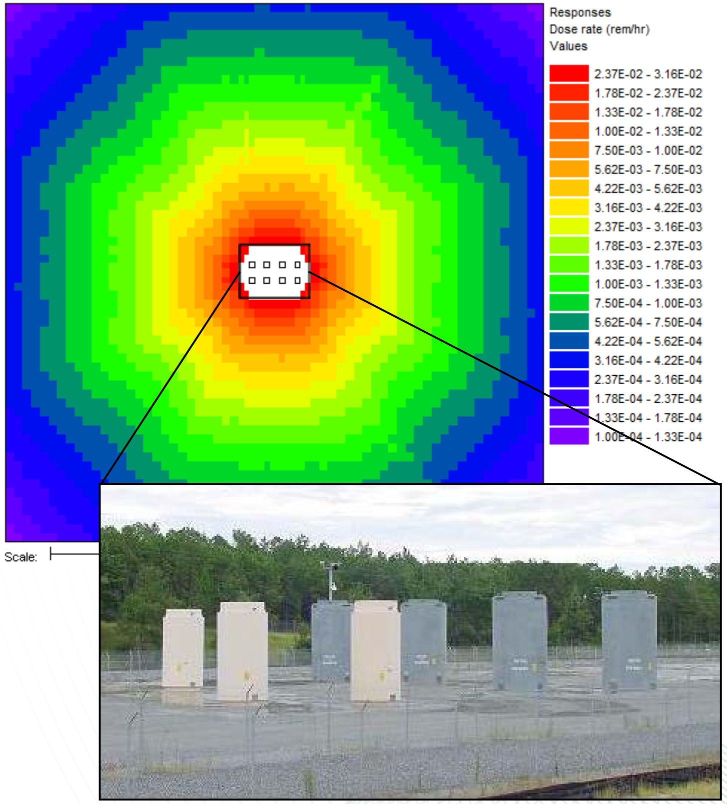
MAVRIC/Monaco Enhancements

- Hybrid deterministic/Monte Carlo shielding and dose assessment tool
- Continuous energy treatment
  - physics, dose responses, tallies
- More/better links to ORIGEN for source terms
  - Read spectrum from binary concentration file
  - Read in photon lines/intensities from ORIGEN data
- Improvements on linking with Denovo
  - Macromaterials for better deterministic models
  - Denovo – more parameters, double precision output
- Improved link with KENO-VI for CAAS Problems
- MAVRIC Utilities – for post-processing

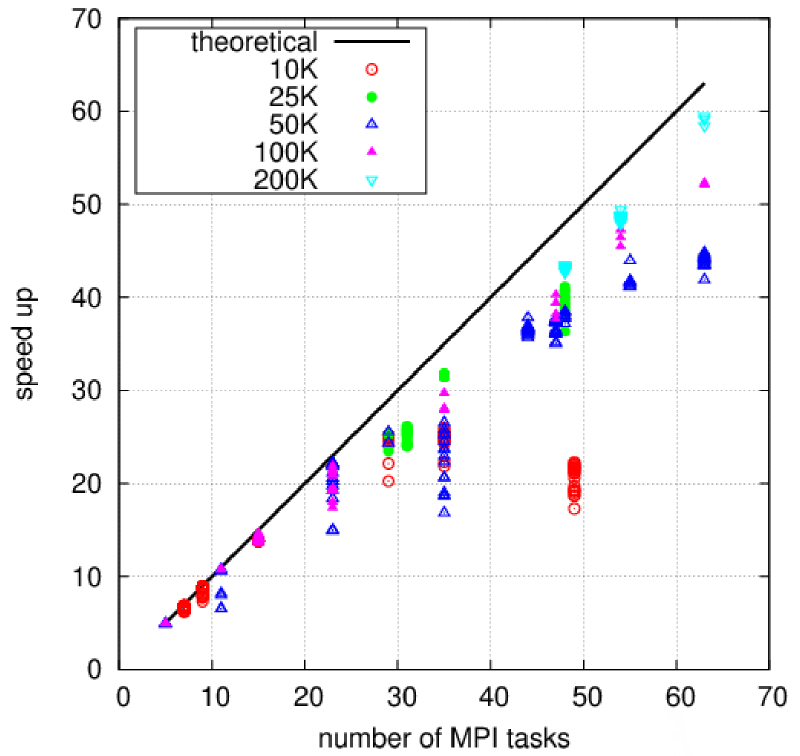


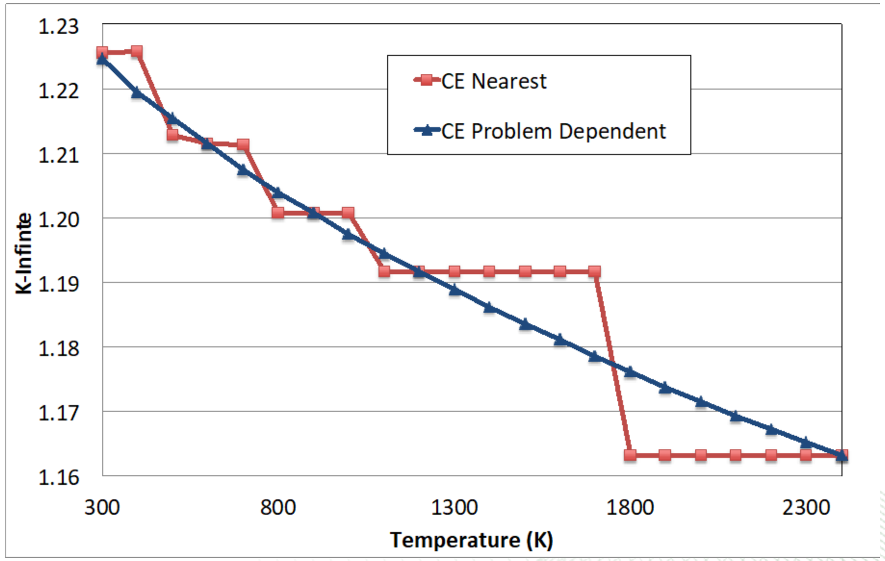
Facility-wide dose assessment



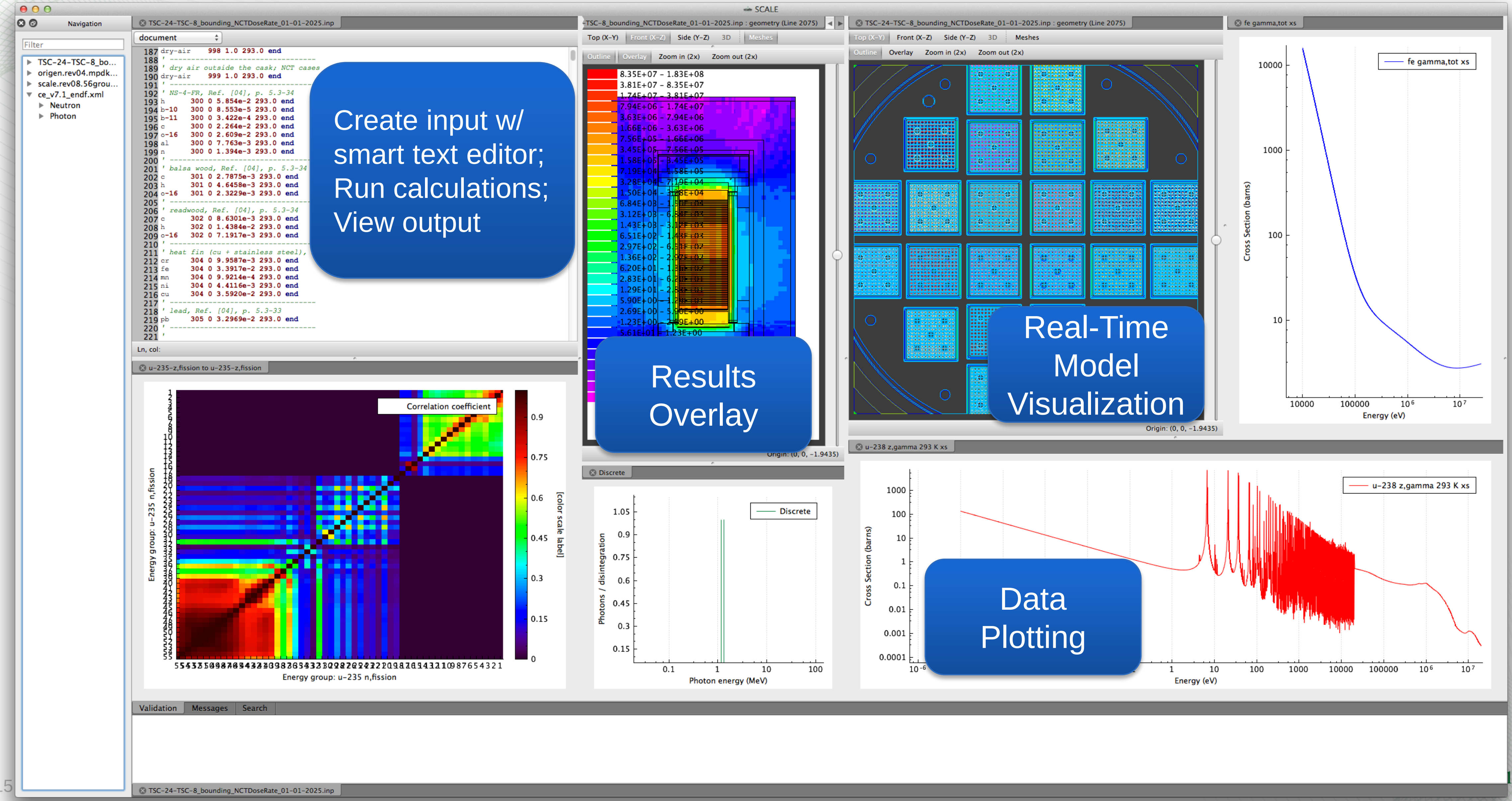
KENO Monte Carlo Enhancements

- Substantial reduction in memory requirements – over 99% improvement in many cases
- Accuracy improvements through comprehensive review and testing
- Parallel Computations
  - Significant speedups with MPI on Linux clusters
- Problem-Dependent Doppler broadening for CE calculations for thermal, resolved, and unresolved energy ranges
- Resonance upscatter treatment
  - Significant improvement in elevated temperature CE Monte Carlo
- Source Convergence
  - Sourcerer – Hybrid sequence to deterministic converge fission source
  - Shannon Entropy diagnostics
- Depletion with ORIGEN for CE and MG



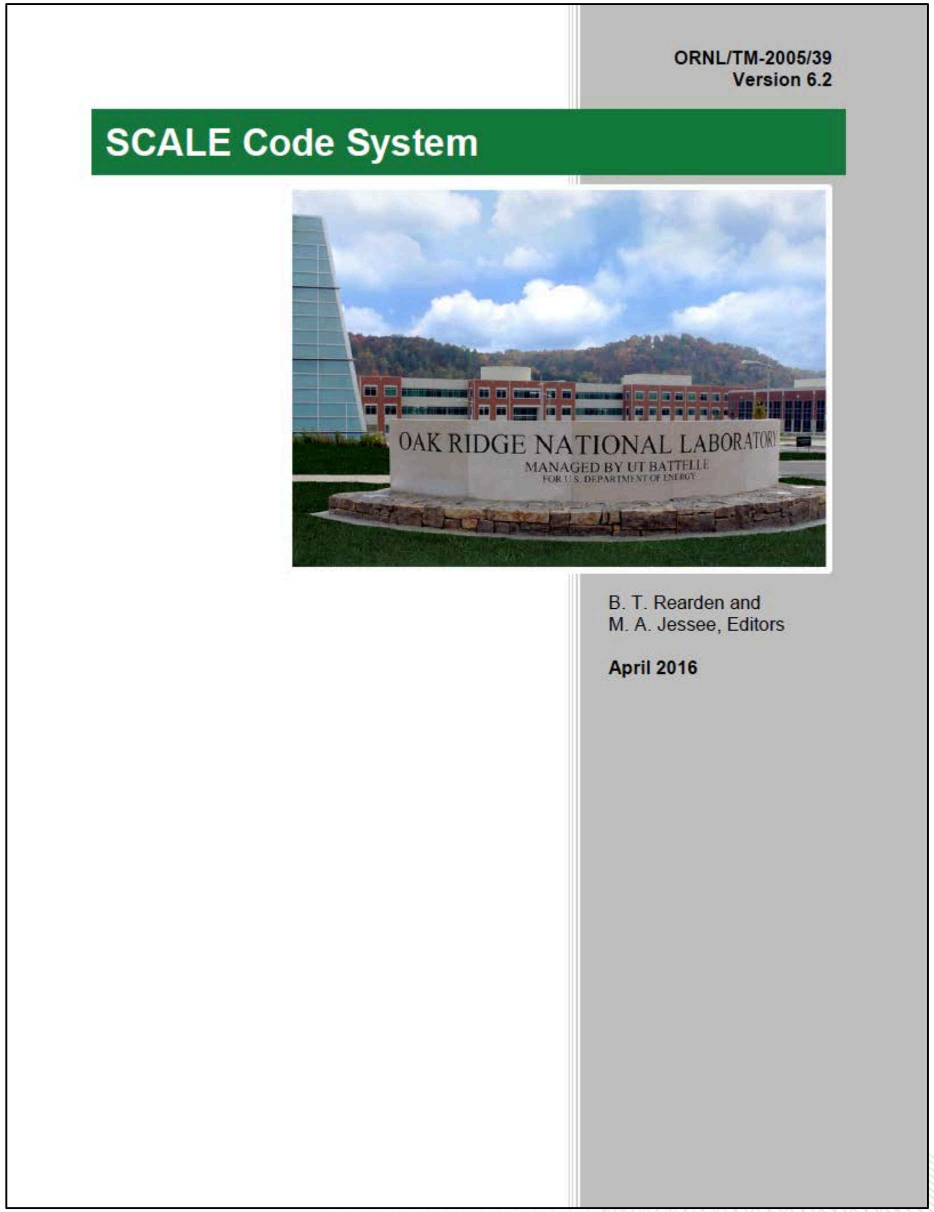


Fulcrum – Integrated User Interface



SCALE documentation has been reorganized and condensed

- SCALE Code System
- README SCALE6.2
- 1.0 Introduction
- 2.0 Criticality Safety
- 3.0 Reactor Physics
- 4.0 Radiation Shielding
- 5.0 Depletion, Activation, and Spent Fuel Source Terms
- 6.0 Sensitivity and Uncertainty Analysis
- 7.0 Material Specification and Cross Section Processing
- 8.0 Monte Carlo Transport
- 9.0. Deterministic Transport
- 10.0 SCALE Nuclear Data Libraries
- 11.0 SCALE Utilities Modules for SCALE Libraries


ORNL/TM-2005/39
Version 6.2

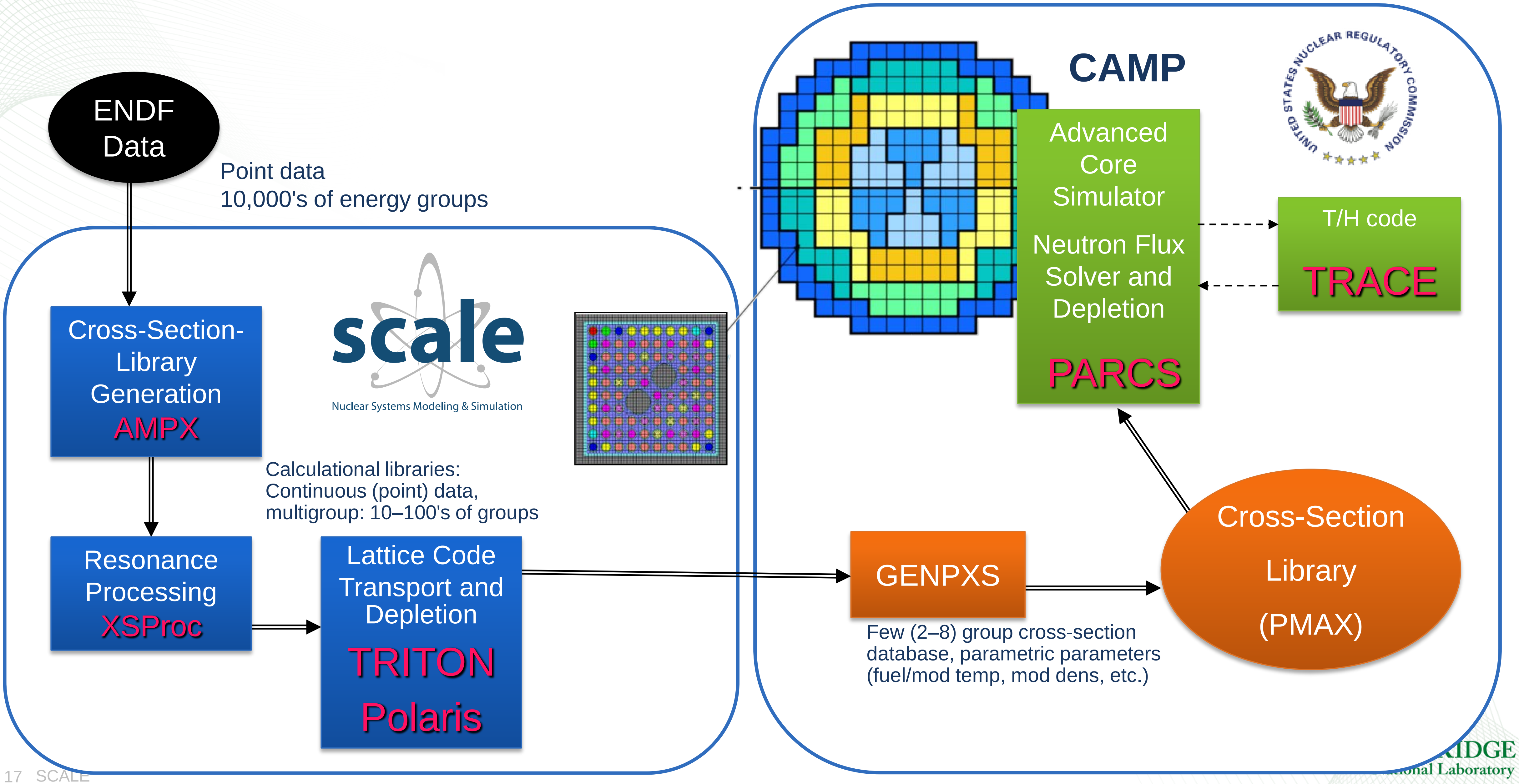
SCALE Code System

B. T. Rearden and
M. A. Jessee, Editors

April 2016

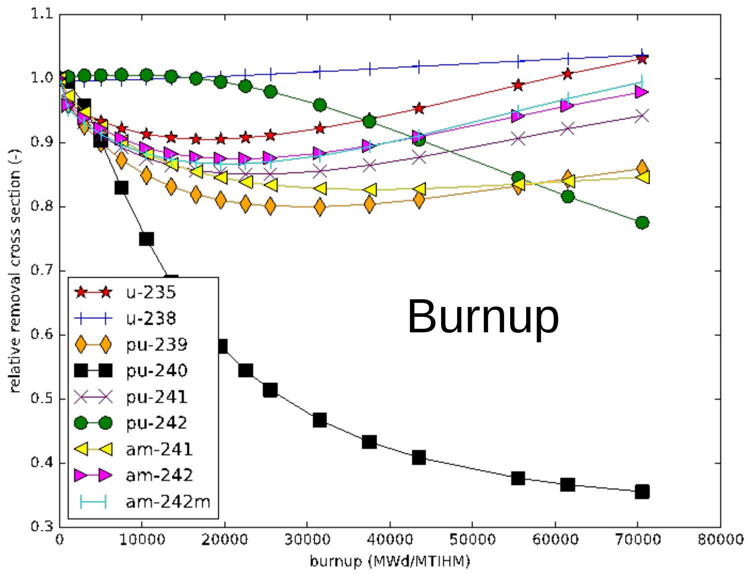
SCALE 6.1: 4894 pages
SCALE 6.2: 2715 pages

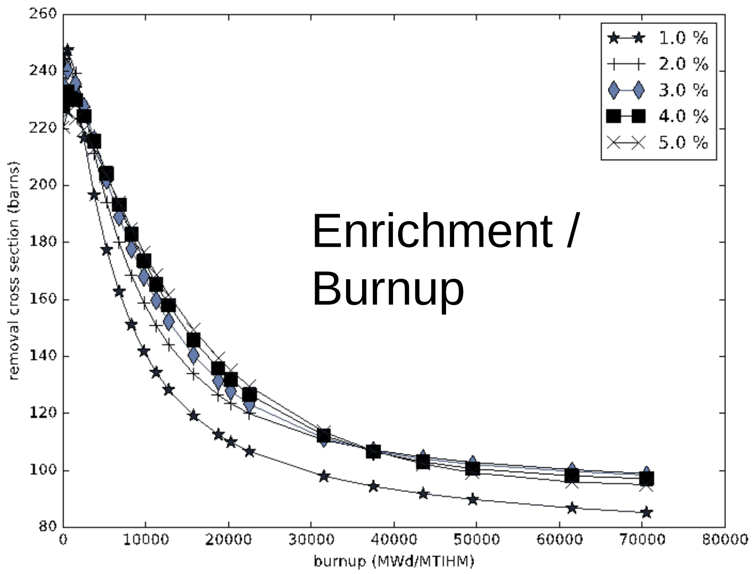
SCALE is a part of NRC's reactor licensing path

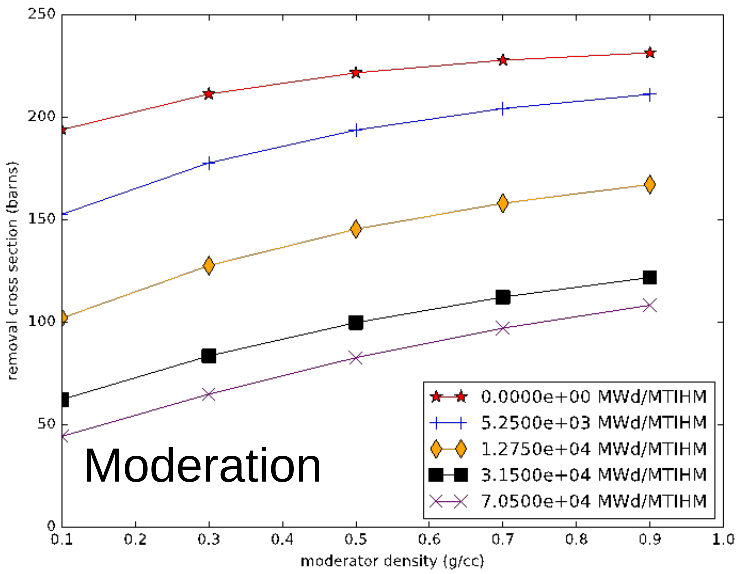


ORIGEN/ORIGAMI Rapid Methodology for Burnup and Source Term Calculations

- Burnup calculation time is limited by flux solve time in assembly/core calculations
- Can pre-compute finite set of burnup calculations covering some space of assembly design/operation to predict isotopics at arbitrary burnups/decay times
- Could create isotopics "database” for many fuel types and conditions, then interpolate
- Better to create cross section "database" and re-solve depletion for the new system (depletion is fast)
- Used by NRC with direct integration with MELCOR/MACCS for severe accident analysis
- Reactor libraries need to be extended to advanced reactors

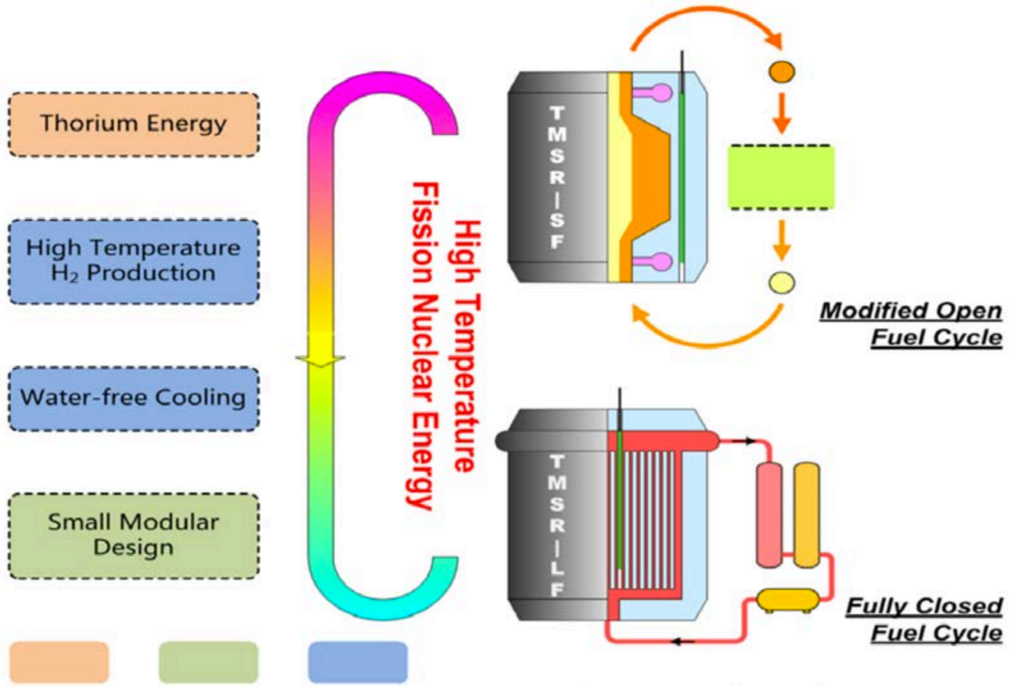






SCALE physics models for TRISO-type fuel particles were updated under CRADA with SINAP

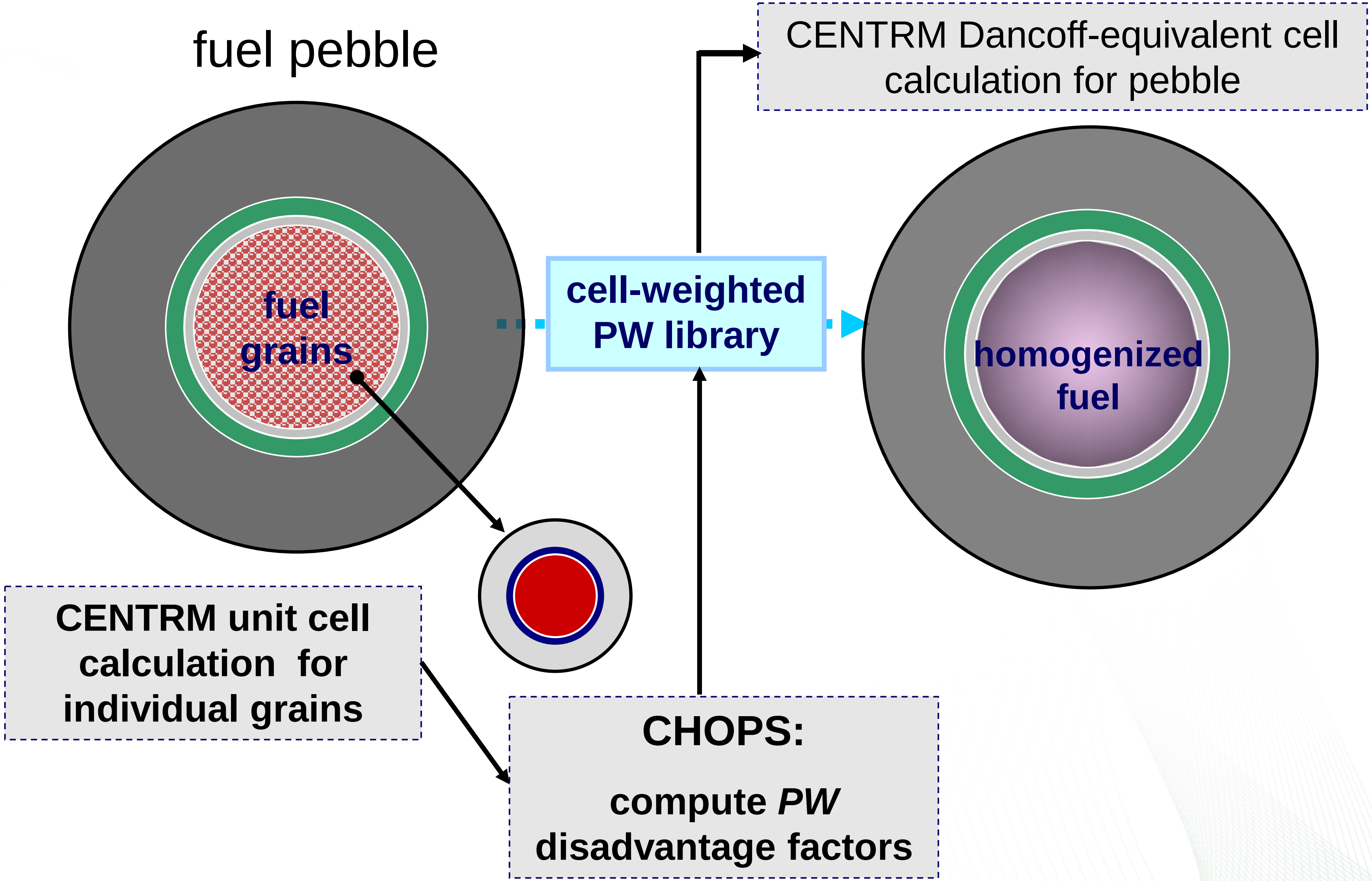
- *"ORNL will update both the continuous-energy and multi-group physics model for TRISO-type fuel particles to improve the flexibility and efficiency of ORNL's SCALE software. The updates would be incorporated within the next release of SCALE."*



Strategy of TMSR R&D

SCALE multigroup double-heterogeneity neutronics

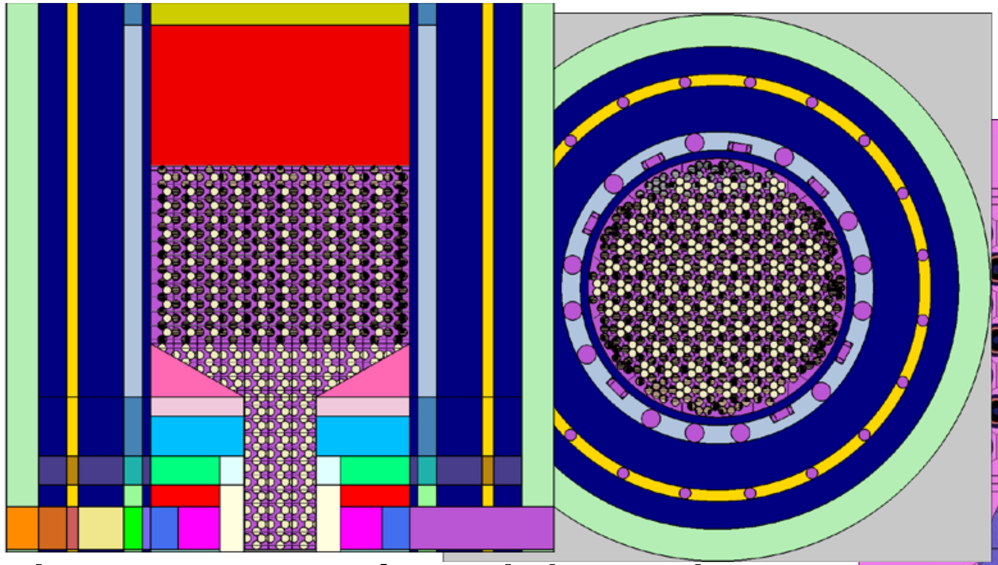
Prior to this work, DoubleHet multigroup TRISO modeling was scheduled for deprecation in SCALE 6.1 due to lack of sponsor support for modernization

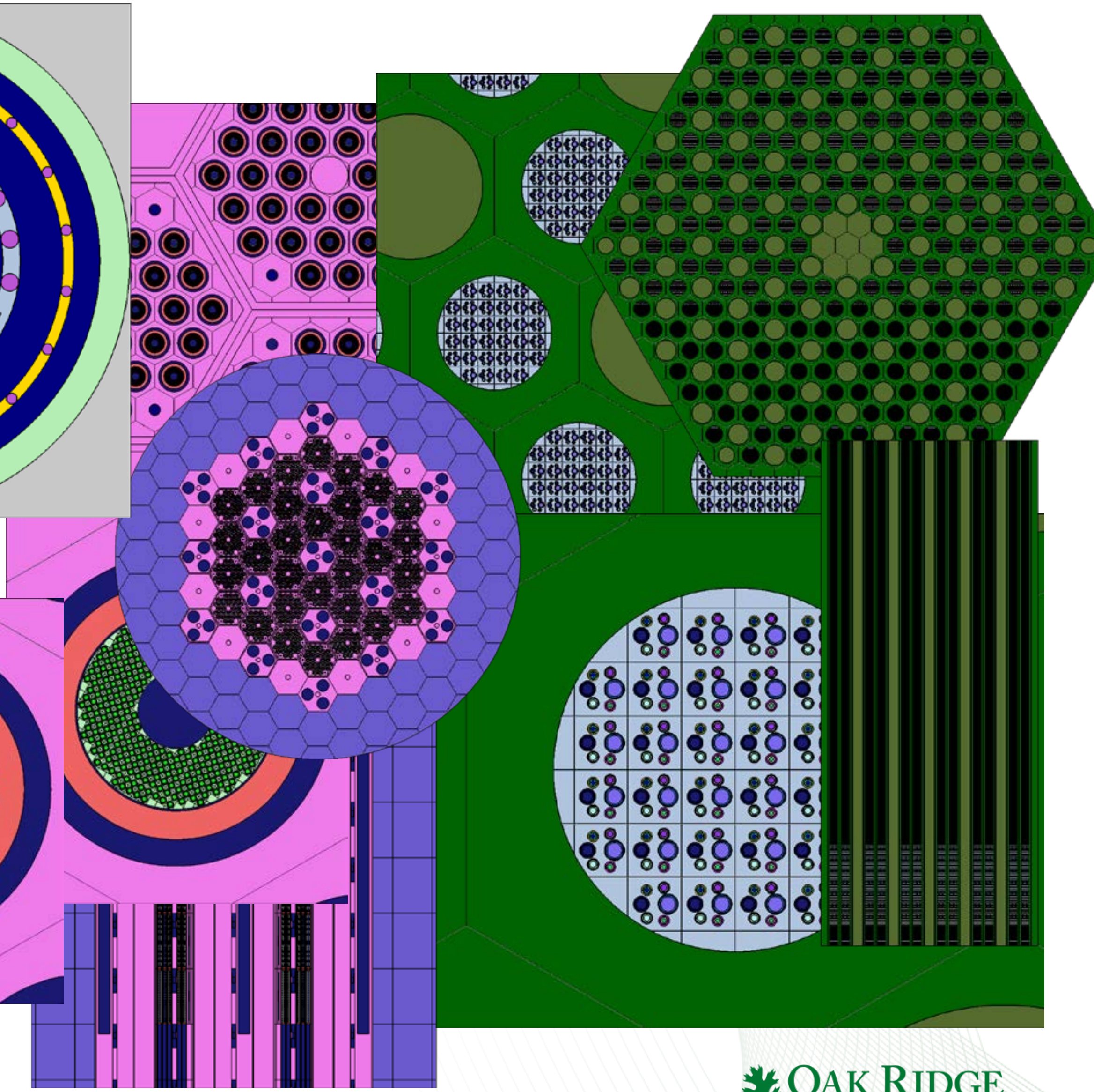


S. Goluoglu and M. L. Williams, "Modeling Doubly Heterogeneous Systems in SCALE," *Trans. Am. Nucl. Soc.* **93**, 963-965 (2005).

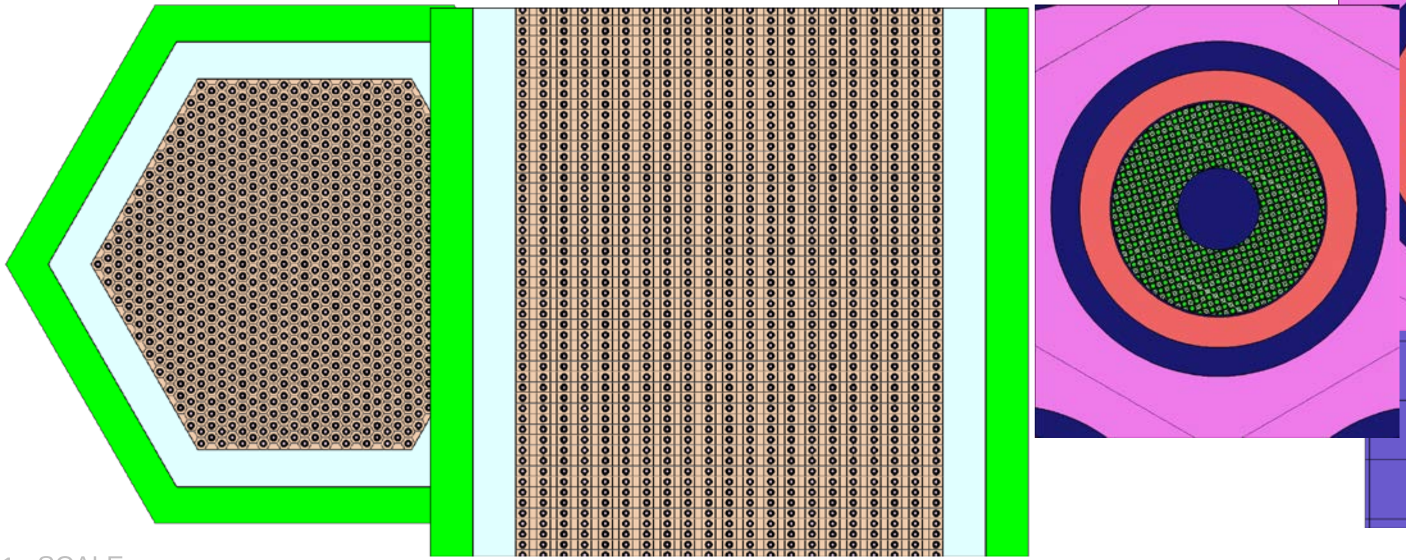
Benchmark models developed for methodology V&V

- HTR-10
- HTTR
- Pebble
- Prismatic
- Fort St. Vrain





- Fully Ceramic Microencapsulated (FCM)



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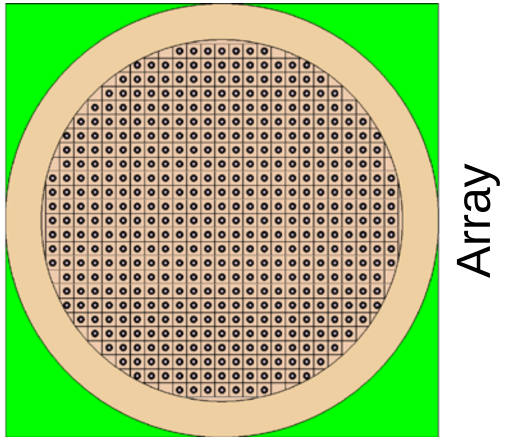
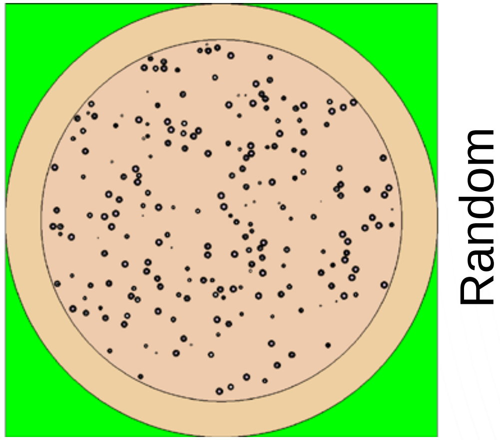
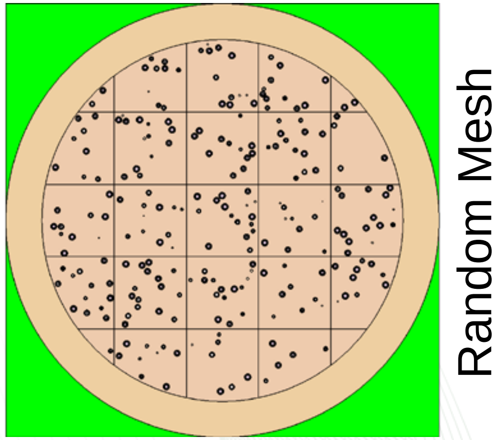
Pebble Models

New Prototype Algorithm for Random Grain Loading

- UO_2 fuel kernel
  - 17 % enriched
  - 8385 kernels/pebble
    - array placement
    - random placement
    - random with mesh placement
- Graphite moderator
- Saturated air coolant
- Reflecting BCs
- ENDF/B-VII.0
  - CE & v7-238







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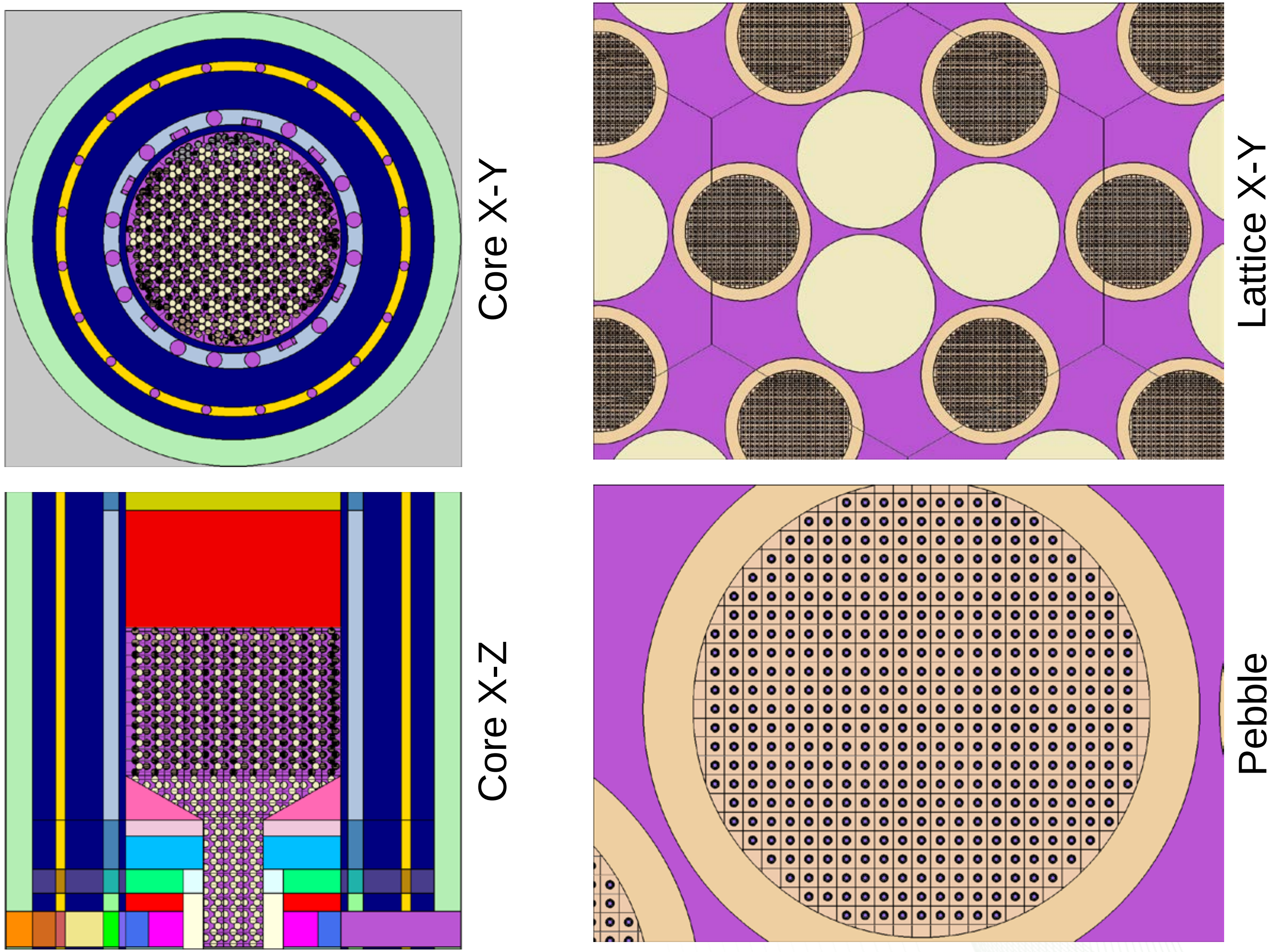
HTR-10 Pebble Results

Code / Modes	k	σ	Δk (pcm)	CPUs	Wall Time (minutes)	Parallel Efficiency	MG Processing Time (minutes)
SCALE 6.2 Continuous-energy Random mesh	1.68314	0.00106	(reference)	75	174 (nearly 3 hours)	97%	-
SCALE 6.2 Continuous-energy Array	1.67900	0.00100	-245	30	4.79	79%	-
SCALE 6.1 Multigroup	1.67406	0.00093	-539	1	7.93	-	1.47
SCALE 6.2 Multigroup	1.68043	0.00098	-161	30	1.18	80%	0.85

HTR-10 Model

- UO_2 fuel kernel
  - 17 % enriched
  - 8385 kernels/pebble
  - array placement
- Graphite moderator
- Saturated air coolant
- ENDF/B-VII.0 cross sections initially used for consistency with earlier work
  - CE & v7-238



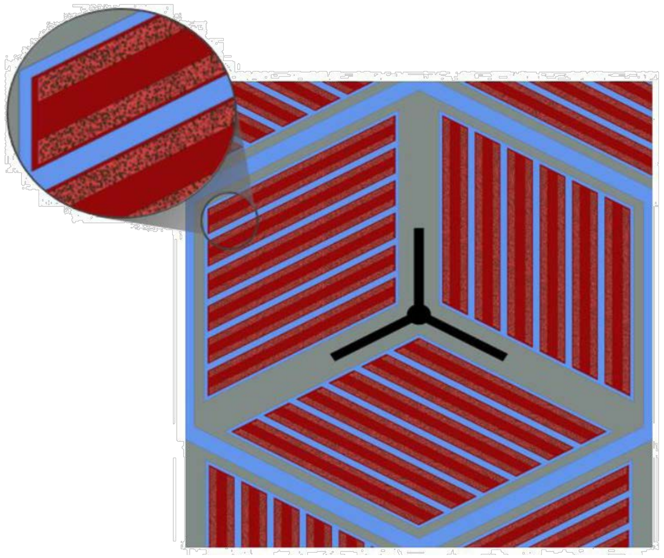
G. Ilas, D. Ilas, R. P. Kelly, and E. E. Sunny, *Validation of SCALE for High Temperature Gas-Cooled Reactor Analysis*, NUREG/CR-7107 (ORNL/TM-2011/161), Oak Ridge National Laboratory, Oak Ridge, Tenn., July 2012.

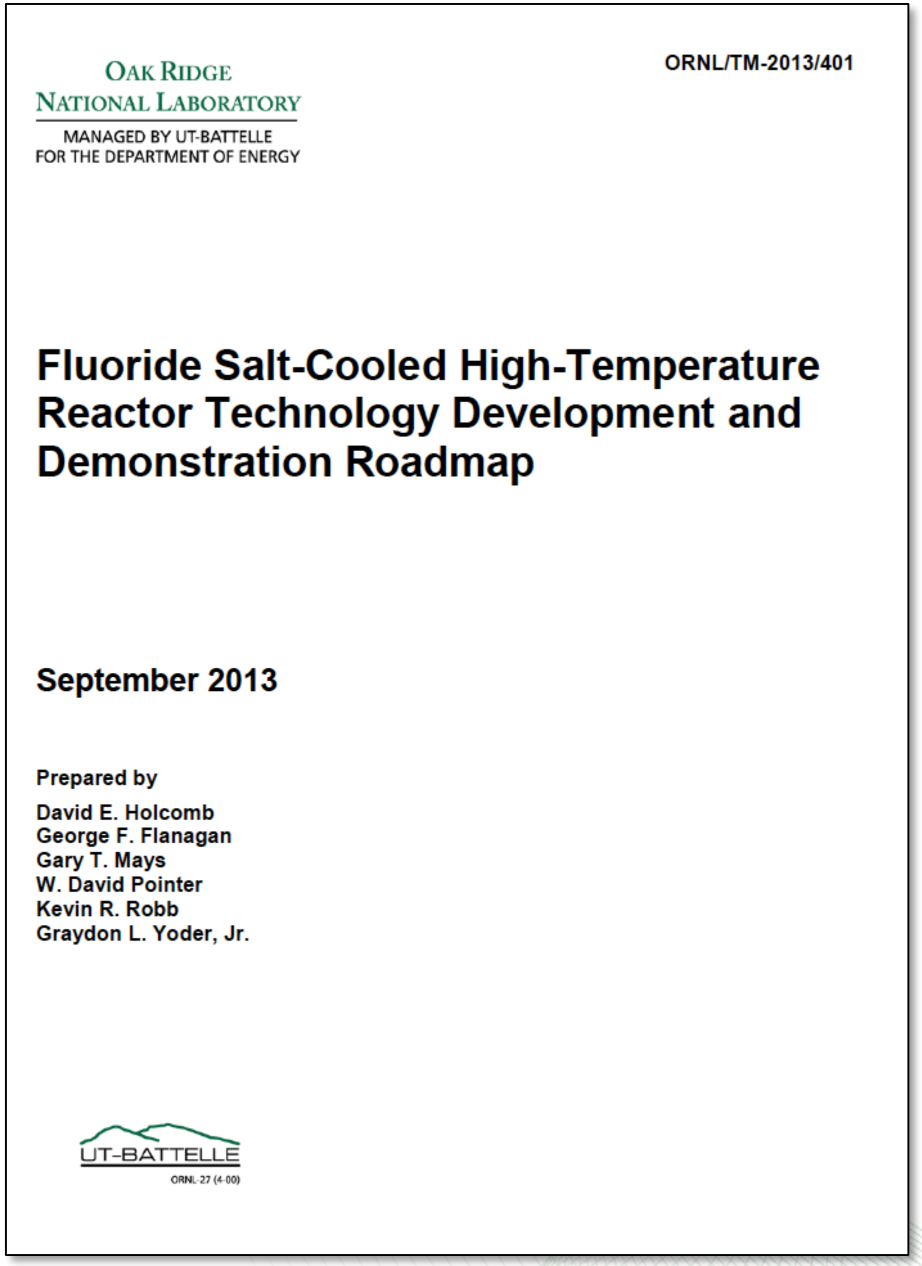
HTR-10 Whole Core Results

Code / Modes	k	σ	Δk (pcm)	CPUs	Wall Time (minutes)	Parallel Efficiency	MG Processing Time (minutes)
SCALE 6.2 Continuous-energy Array	1.01412	0.00032	(reference)	30	254	82%	
SCALE 6.1 Multigroup	1.01487	0.00027	74	1	2178 (36 hours)	-	4.87
SCALE 6.2 Multigroup	1.01623	0.00025	208	30	63	88%	3.88

Support for Additional Fuel Geometries

- All previous versions of SCALE only supported DoubleHet modeling of cylindrical and spherical fuel designs
- Several teams have spend a great amount of effort working around this deficiency





OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

ORNL/TM-2013/401

Fluoride Salt-Cooled High-Temperature Reactor Technology Development and Demonstration Roadmap

September 2013

Prepared by

David E. Holcomb
George F. Flanagan
Gary T. Mays
W. David Pointer
Kevin R. Robb
Graydon L. Yoder, Jr.

UT-BATTELLE

ORNL-27 (4-00)

DoubleHet Fuel Lattice Types Supported in SCALE 6.2

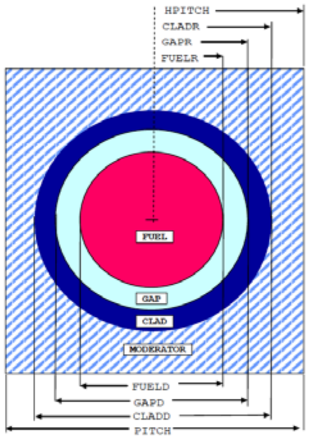


Figure 7.1.1. Arrangement of materials in a SQUAREPITCH and SPHSQUAREP unit cell.

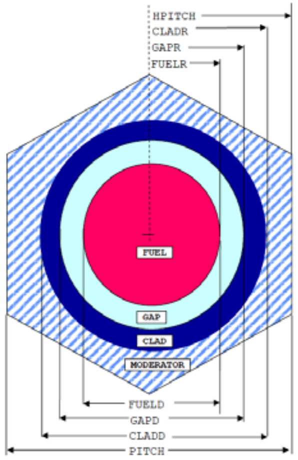


Figure 7.1.2. Arrangement of materials in a TRIANGPITCH and SPHTRIANGP unit cell.

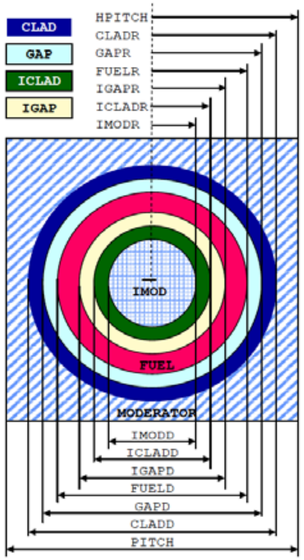


Figure 7.1.4. Arrangement of materials in an ASQUAREPITCH and ASPHSQUAREP unit cell.

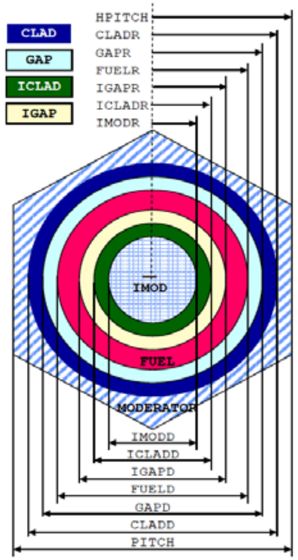


Figure 7.1.5. Arrangement of materials in an ATRIANGPITCH and ASPHTRIANGP unit cell.

Regular Cells

SQUAREPITCH (available in 6.1) is used for an array of cylinders arranged in a square lattice, as shown in Figure 7.1.1. The clad and/or gap can be omitted.

TRIANGPITCH (available in 6.1) is used for an array of cylinders arranged in a triangular-pitch lattice as shown in Figure 7.1.2. The clad and/or gap can be omitted.

SPHSQUAREP (available in 6.1) is used for an array of spheres arranged in a square-pitch lattice. A cross section view through a cell is represented by Figure 7.1.1. The clad and/or gap can be omitted.

SPHTRIANGP (available in 6.1) is used for an array of spheres arranged in a triangular-pitch (dodecahedral) lattice. A cross section view through a cell is represented by Figure 7.1.2. The clad and/or gap can be omitted.

SYMMSLABCELL is used for an infinite array of symmetric slab cells, as shown in Figure 7.1.3. The clad and/or gap can be omitted.

Annular Cells

ASQUAREPITCH or **ASQP is used for annular cylindrical rods in a square-pitch lattice as shown in** Figure 7.1.4. The inner and outer clad and gap are independently entered so they may be different materials and dimensions.

ATRIANGPITCH or **ATRP is used for annular cylindrical rods in a triangular-pitch lattice as shown in** Figure 7.1.5. The inner and outer clad and gap are independently entered, so they may be different materials and dimensions.

ASPHSQUAREP or **ASSP is used for spherical shells in a square-pitch lattice as shown in** Figure 7.1.4. The inner and outer clad and gap are independently entered, so they may be different materials and dimensions.

ASPHTRIANGP or **ASTP is used for spherical shells in a triangular-pitch (dodecahedral) lattice as shown in** Figure 7.1.5. The inner and outer clad and gap are independently entered, so they may be different materials and dimensions.

ASYMSLABCELL is used for a periodic, but asymmetric, array of slabs as shown in Figure 7.1.6. The inner and outer clad and gap are independently entered, so they may be different materials and dimensions.

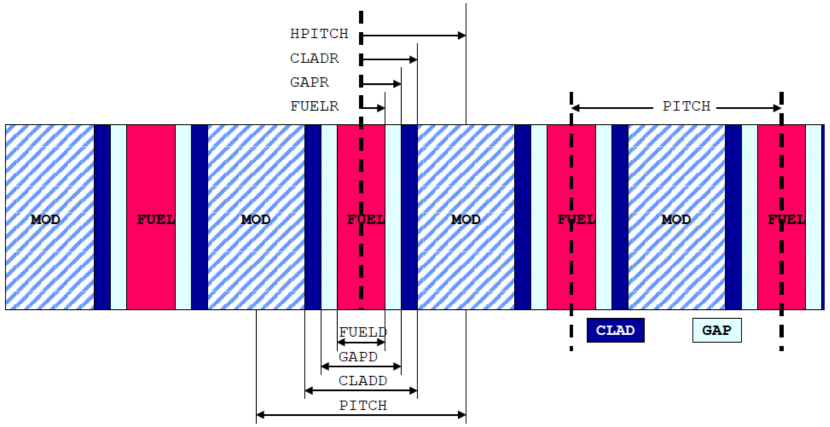


Figure 7.1.3. Arrangement of materials in a SYMMSLABCELL unit cell having reflected left and right boundary conditions.

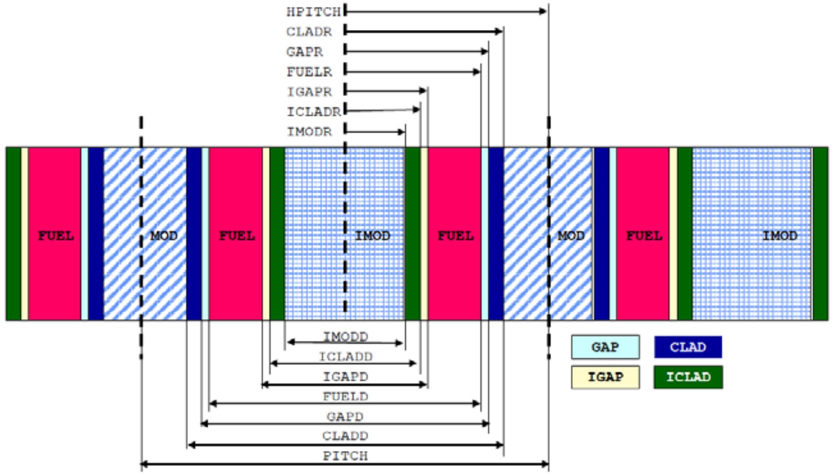


Figure 7.1.6. Arrangement of materials in an ASYMSLABCELL unit cell having reflected left and right boundary conditions.

Carbon activation/depletion with ENDF/B-VII.1

- ENDF only provides cross sections for elemental C (not C-12, C-13, C-14)
- Isotopes for depletion are available in JEFF activation library, so TRITON was updated for a special case to map the data appropriately
- Natural abundances and nuclear masses were outdated in ORIGEN libraries, so was ORIGEN updated to draw data from SCALE Standard Composition Library
- Updated for SCALE 6.2

Nuclide	Initial loading	SCALE 6.2
	g/MTU	g/MTU
C-12	2.4953E+04	2.4952E+04
C-13	2.6988E+02	2.9998E+02
C-14	0	2.0096E-03

Note that the results above were based on burnup of 40 GWd/MTU

Tritium production in SCALE

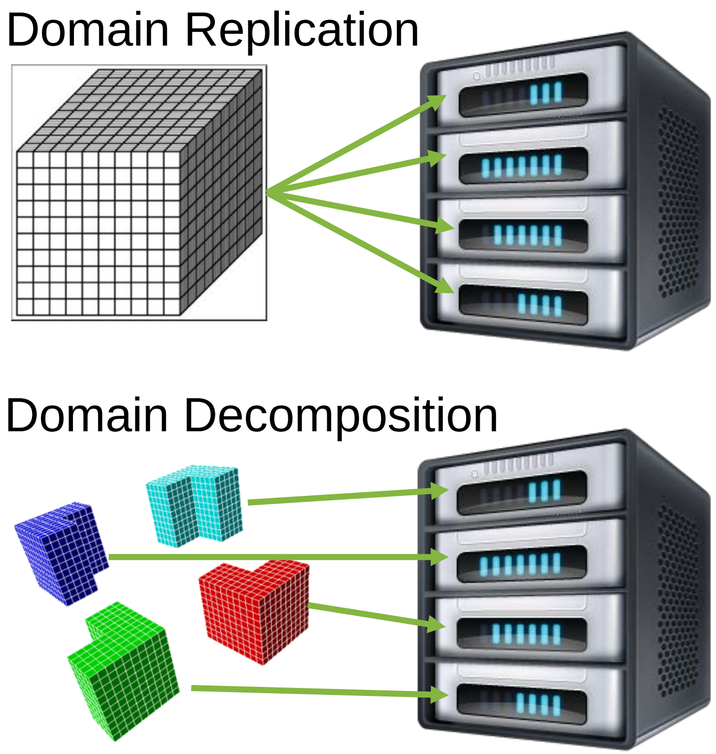
- Tritium is safety concern for some MSRs because lithium-activation produces orders of magnitude higher amounts of tritium than LWRs
- Tritium production physics have been improved in SCALE 6.2
- Validated with MSRE benchmark data: R. B. Briggs, "Tritium in Molten-Salt Reactors," *Reactor Technology*, **14(4)**:335 (Winter 1971-1972)

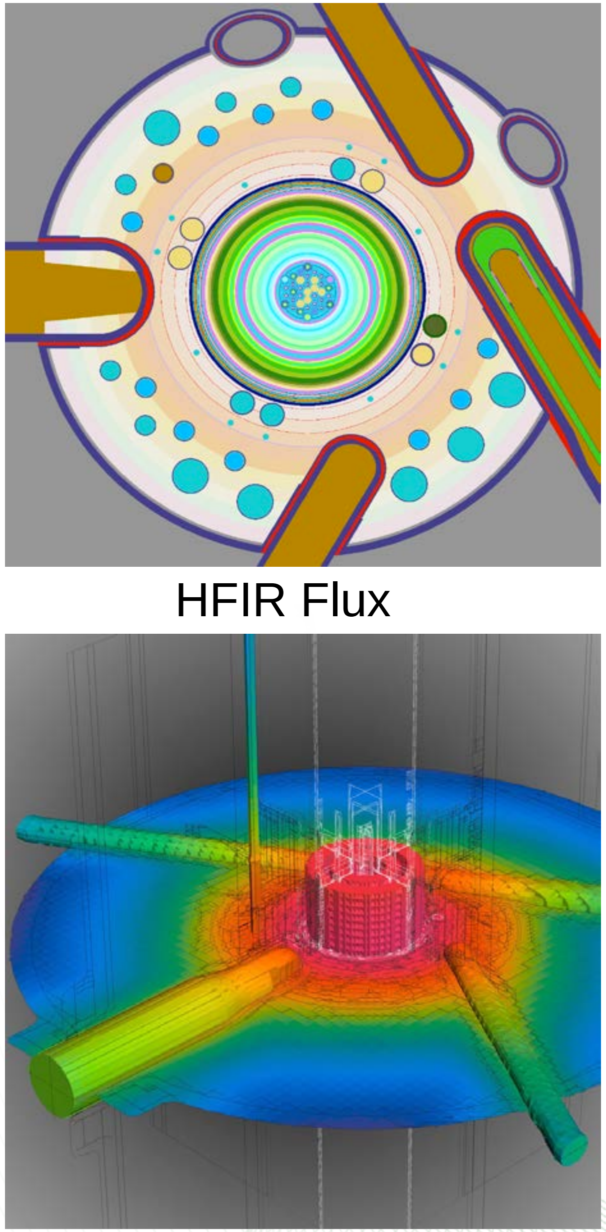
Nuclide	Measured (Ci/MTU)	SCALE 6.2 (Ci/MTU)	C/E
H-3	8.12E+04	1.11E+05	1.37

Note that the SCALE results above were based constant irradiation of 375 days with specific power of 30 MW/MTU to simulate the tritium production of ORNL MSRE. Enrichment of Li-7 is 99.99%. <u>SCALE 6.2 results agree within precision of experimental measurement.</u>

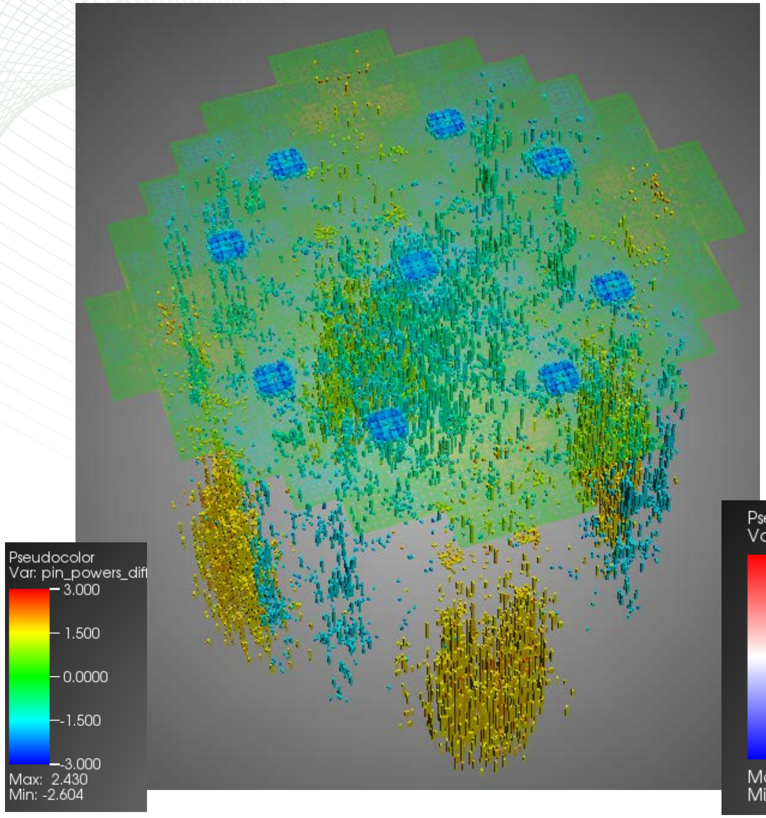
Advanced reactor Monte Carlo analysis with Shift

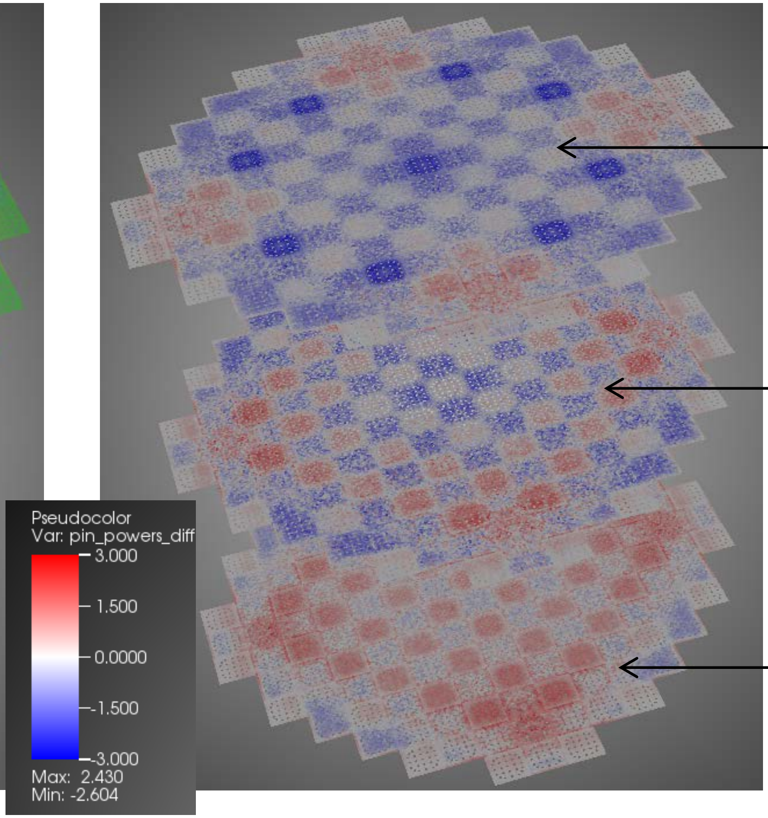
- Flexible, high-performance Monte Carlo radiation transport *framework*
- Shift is physics agnostic
  - SCALE CE physics
  - SCALE MG physics
- Shift is geometry agnostic
  - SCALE geometry
  - Exnihilo RTK geometry
  - MCNP geometry
  - DagMC-CUBIT CAD geometry
- Fixed-source and eigenvalue solvers
- Integrated with Denovo for hybrid methods
- Multiple parallel decompositions and concurrency models
- Shift is designed to scale from supercomputers to laptops





Shift provides reference solutions for CASL



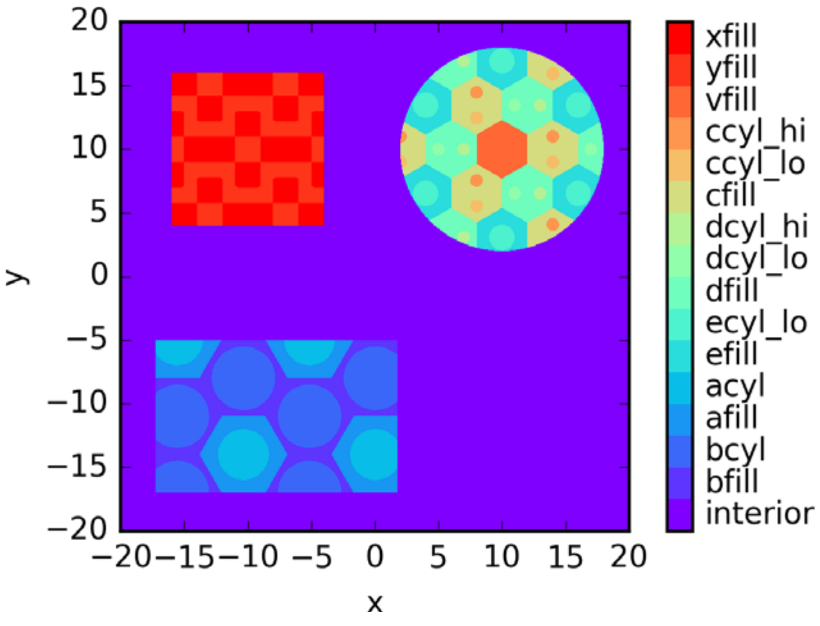


- Shift – generated reference solutions provide benchmarks for VERA-CS
- HPC scalability of Shift enables the highest resolution possible solutions of 3D LWR cores using OLCF resources (Titan)
- Integration with VERA allows analysts to generate benchmarks from the same inputs and models as production runs

Case	Bank Position (% Inserted)	AO (%)	ΔAO (%) MPACT	RMS ΔP (%) MPACT	Max ΔP (%) MPACT
3x3 Reg. B and D	AO, 17% In	-7.5	-0.1	0.4	1.9
Quarter Core	AO, 17% In MD, 66% In MC, 100% In	-8.7	+0.2	0.6	2.6

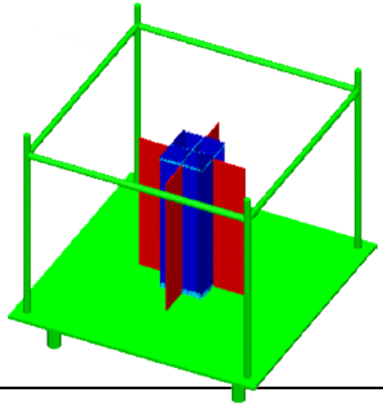
Shift / SCALE Integration

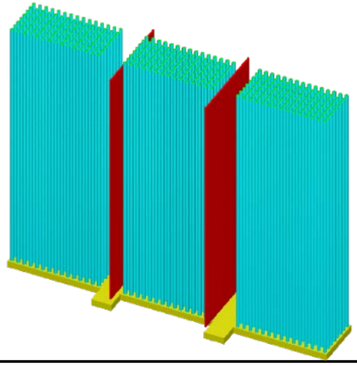
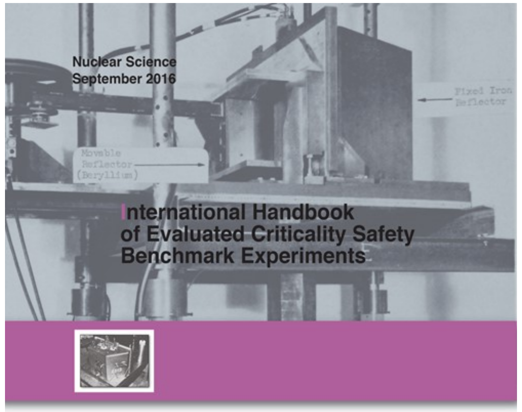
- **Integrated in CSAS criticality sequence**
  - Eigenvalue mode for criticality safety
  - Uses standard SCALE geometry, material, and control specifications
- **Integration in TRITON lattice-physics**
  - Currently in-development
  - Flux-solver
  - Depletion
  - Multigroup cross section generation for nodal codes
  - Randomize geometry for TRISO and pebble bed
- **Integration in TSUNAMI**
  - Capability demonstrated
  - Eigenvalue and generalized perturbation theory sensitivity coefficients with CE physics
- **Integration in MAVRIC**
  - Fixed-source shielding problems using hybrid methods especially for large facility and site modeling
  - Planned for future development



Validation with critical benchmarks for many types of systems

- 411 configurations from International Criticality Safety Benchmark Evaluation Project (ICSBEP)

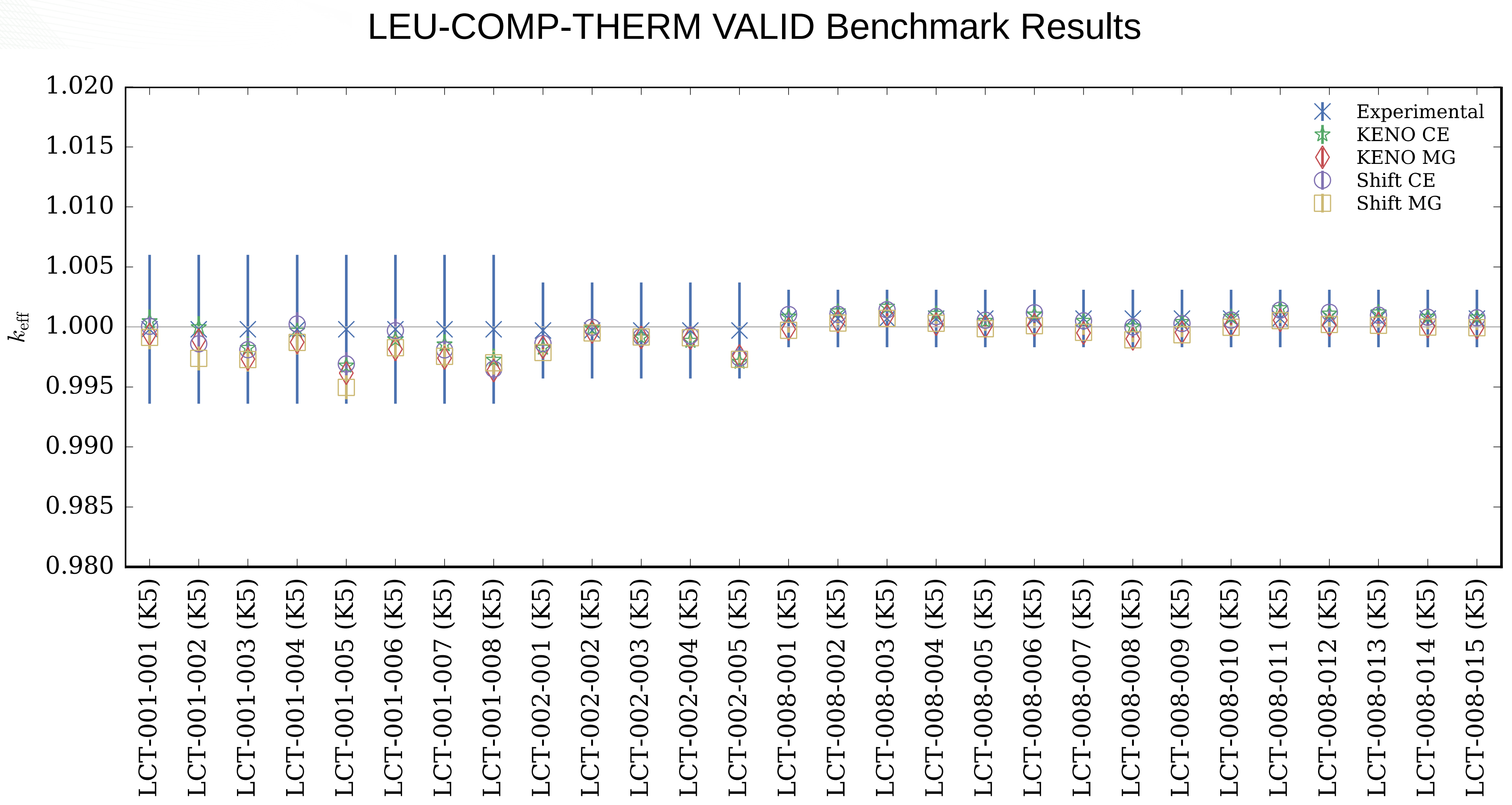



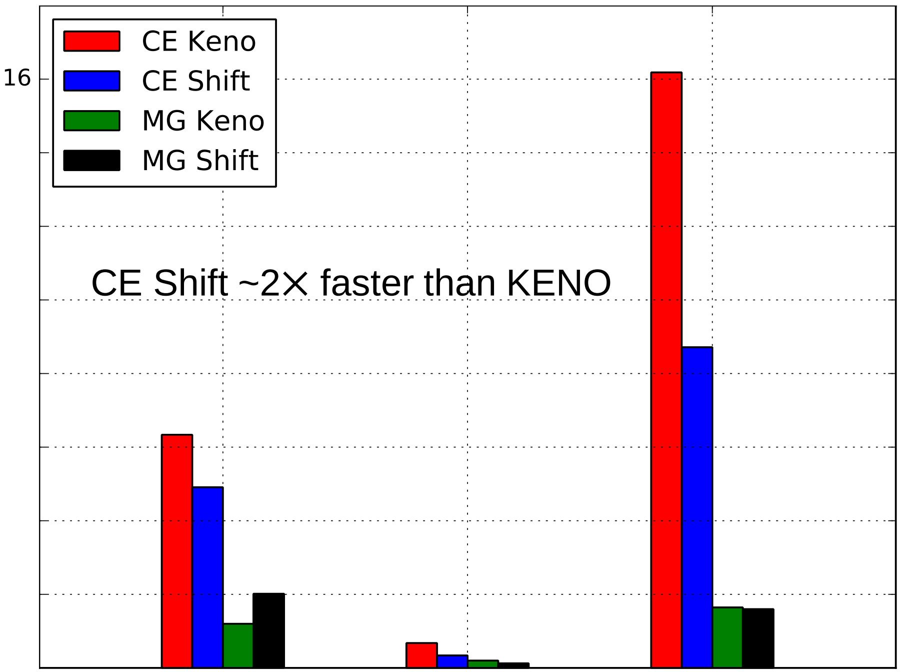
Sequence / Geometry	Experiment class	ICSBEP case numbers	Number of configurations
CSAS5 / KENO V.a	HEU-MET-FAST	15, 16, 17, 18, 19, 20, 21, 25, 30, 38, 40, 65	18
	HEU-SOL-THERM	1, 13, 14, 16, 28, 29, 30	52
	IEU-MET-FAST	2, 3, 4, 5, 6, 7, 8, 9	8
	LEU-COMP-THERM	1, 2, 8, 10, 17, 42, 50, 78, 80	140
	LEU-SOL-THERM	2, 3, 4	19
	MIX-MET-FAST	5, 6	2
	MIX-COMP-THERM	1, 2, 4	21
	MIX-SOL-THERM	2	3
	PU-MET-FAST	1, 2, 5, 6, 8, 10, 18, 22, 23, 24	10
	PU-SOL-THERM	1, 2, 3, 4, 5, 6, 7, 11, 20	81
CSAS6 / KENO-VI	HEU-MET-FAST	5, 8, 9, 10, 11, 13, 24, 80, 86, 92, 93	27
	IEU-MET-FAST	19	2
	MIX-COMP-THERM	8	28

- **Fissile materials**
  - High-enriched uranium (HEU),
  - Intermediate-enriched uranium (IEU)
  - Low-enriched uranium (LEU)
  - Plutonium (Pu)
  - Mixed uranium/plutonium oxides (MOX)
- **Fuel form**
  - Metal (MET),
  - Fissile solution (SOL)
  - Multi-material composition (e.g. fuel pins – COMP)
- **Neutron spectra**
  - Fast
  - Thermal

Scale-Shift Validation (ORNL/SR-2016/401)

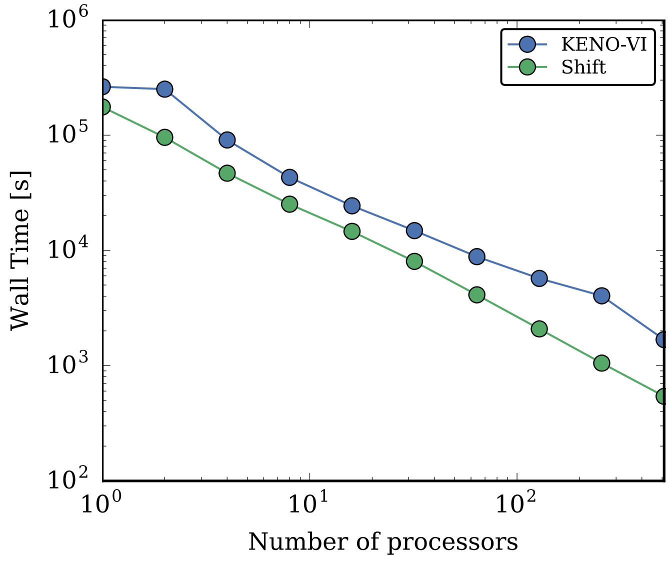


SCALE-Shift Performance

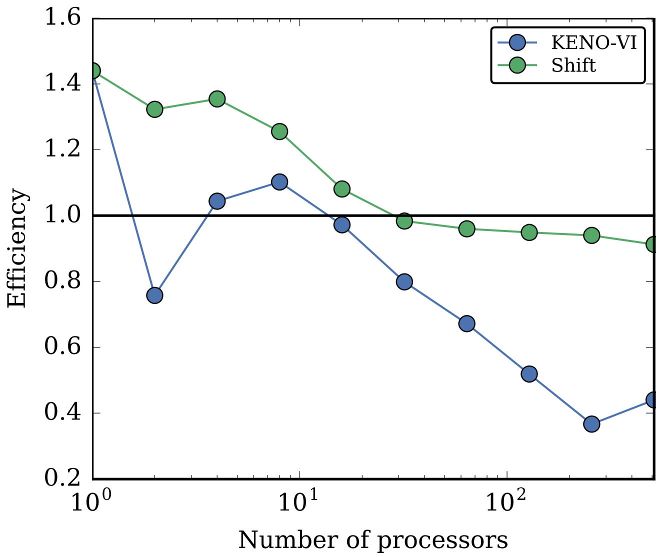


Serial Runtimes

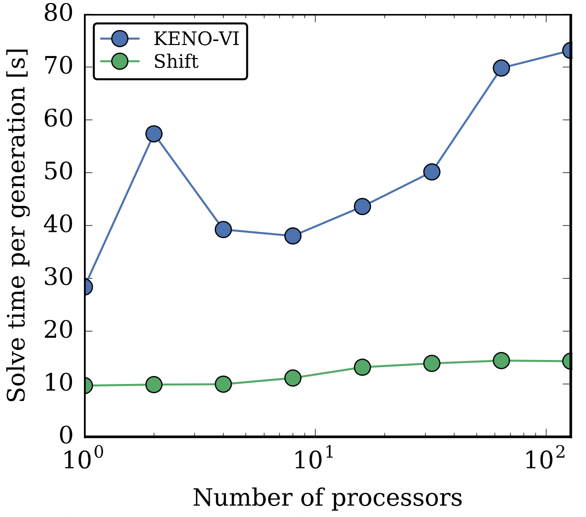
Industry-Scale Parallel Performance



Strong Scaling



Weak Scaling



OAK RIDGE National Laboratory

SCALE enhancements for advanced reactor analysis

- SCALE 6.2
  - Parallel CE Monte Carlo w/ Doppler broadening
    - criticality
    - depletion
    - sensitivity/uncertainty
  - AMPX codes to generate cross section libraries
  - Sensitivity/uncertainty tools and data
  - Efficient hybrid methods for facility and site dose rate assessment
  - Fulcrum user interface
  - Enhanced double-heterogeneity treatments
  - Carbon activation/depletion
  - Tritium production

- Emerging capabilities
  - Advanced Monte Carlo capabilities with Shift for
    - criticality
    - depletion
    - shielding
    - sensitivity/uncertainty
    - nodal cross section generation
    - randomized geometry
  - Cross section libraries optimized for advanced reactors
  - Advanced methods for double-heterogeneity fuels
  - Source term reactor libraries extended for advanced reactors
  - Validation and uncertainty analysis for advanced reactors

scale
Nuclear Systems Modeling & Simulation

An Introduction to NEAMS Workbench

Brad Rearden (ORNL)

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

NEAMS Workbench

Bradley T. Rearden, Ph.D.
Leader, NEAMS Integration Product Line

Robert A. Lefebvre
Leader, Workbench Development
Oak Ridge National Laboratory

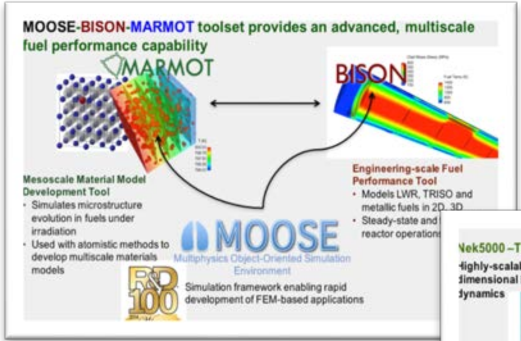
Workshop on Tools for Modeling and Simulation of Fluoride Cooled High Temperature Reactors (FHR)
Georgia Institute of Technology
February 8-9, 2017

NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

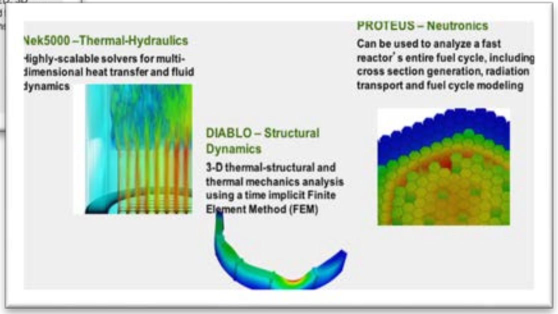
U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NEAMS (Nuclear Energy Advanced Modeling and Simulation) Program

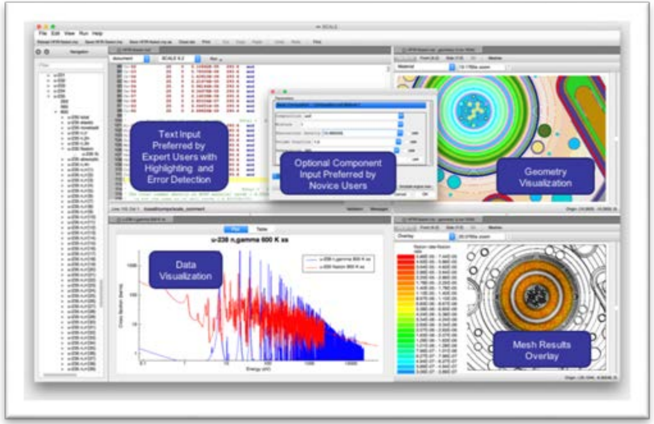
Aim: Develop, apply, deploy, and support a predictive modeling and simulation toolkit for the design and analysis of current and future nuclear energy systems using computing architectures from laptops to leadership class facilities.



Fuels Product Line



Reactor Product Line



Integration Product Line

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NEAMS Organizational Structure

Leadership Council

National Technical Director
Chris Stanek (LANL)

Project: Accident Tolerant Fuels
Jason Hales (INL)

Fuels Product Line
Steve Hayes (INL)

Integration Product Line
Brad Rearden (ORNL)

Reactors Product Line
Tanju Sofu (ANL)

Project: Steam Generator Flow Induced Vibration
Elia Merzari (ANL)

Shane Johnson
Deputy Assistant Secretary, Science and Technology Innovation(NE-5)

Tom Miller
Office of Accelerated Innovation in Nuclear (NE-51)

Dan Funk
National Laboratory and Industry Capabilities Team (NE-51.1)

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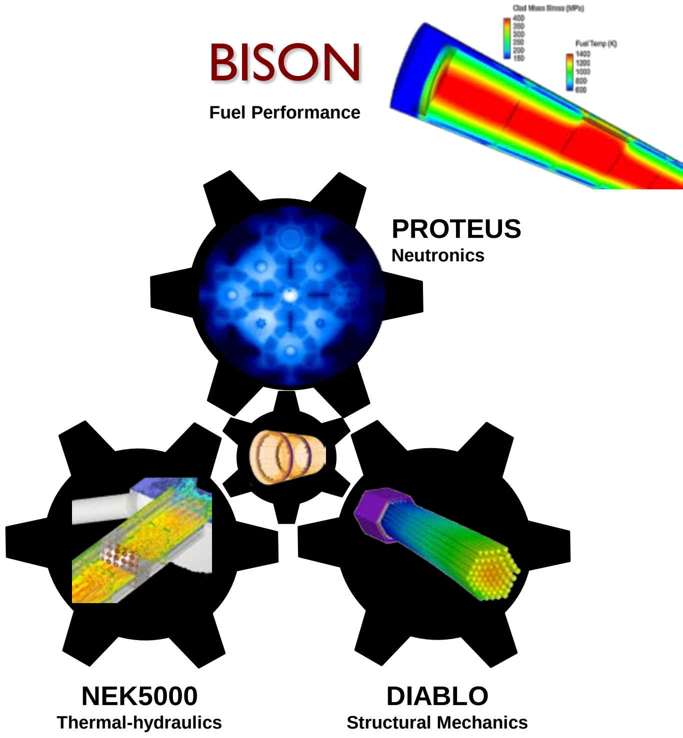
Integration Product Line (IPL)

- **NEAMS Fuels Product Line (FPL) and Reactors Product Line (RPL) provide many advanced tools, but they often require large computational resources, can be difficult to install, and require expert knowledge to operate, causing many analysts to continue to use traditional tools instead of exploring high-fidelity simulations.**

- **Goal: Respond to needs of design and analysis communities by integrating robust multiphysics capabilities and current production tools in easy-to-use versioned deployments that enable end users to apply high-fidelity simulations to inform lower-order models for the design, analysis, and licensing of advanced nuclear systems.**



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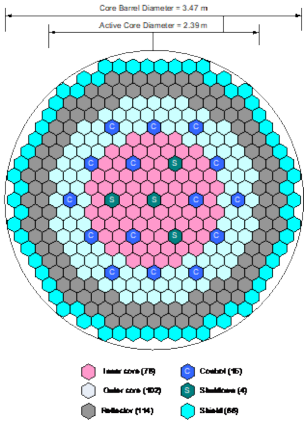
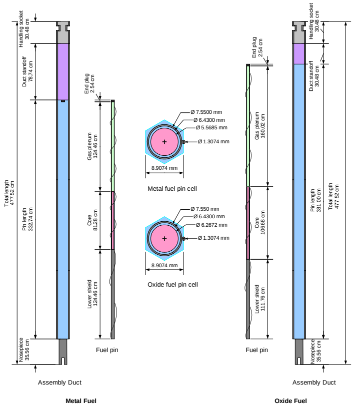
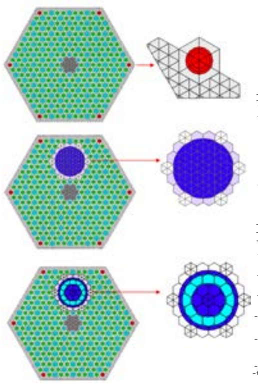
Fast Reactor Analysis Codes from Advanced Reactor Technologies Program

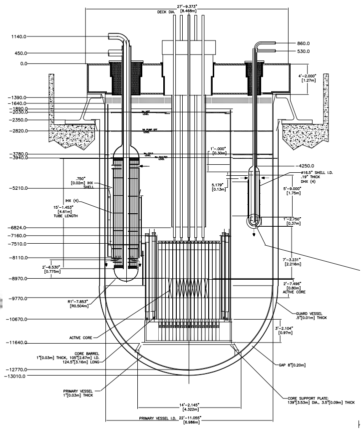




Workbench

- Input creator and code flow management
- Ease transition to new high-fidelity codes
- Ensures best-practice and ease of utilization
- Ideal for training and deployment





MC²-3 | *DIF3D* | *REBUS* | *PERSENT* | *SE2-ANL* | *LIFE-METAL* | *SAS4A* | *New function.*

MCNP | *ORIGEN* | *New tools*

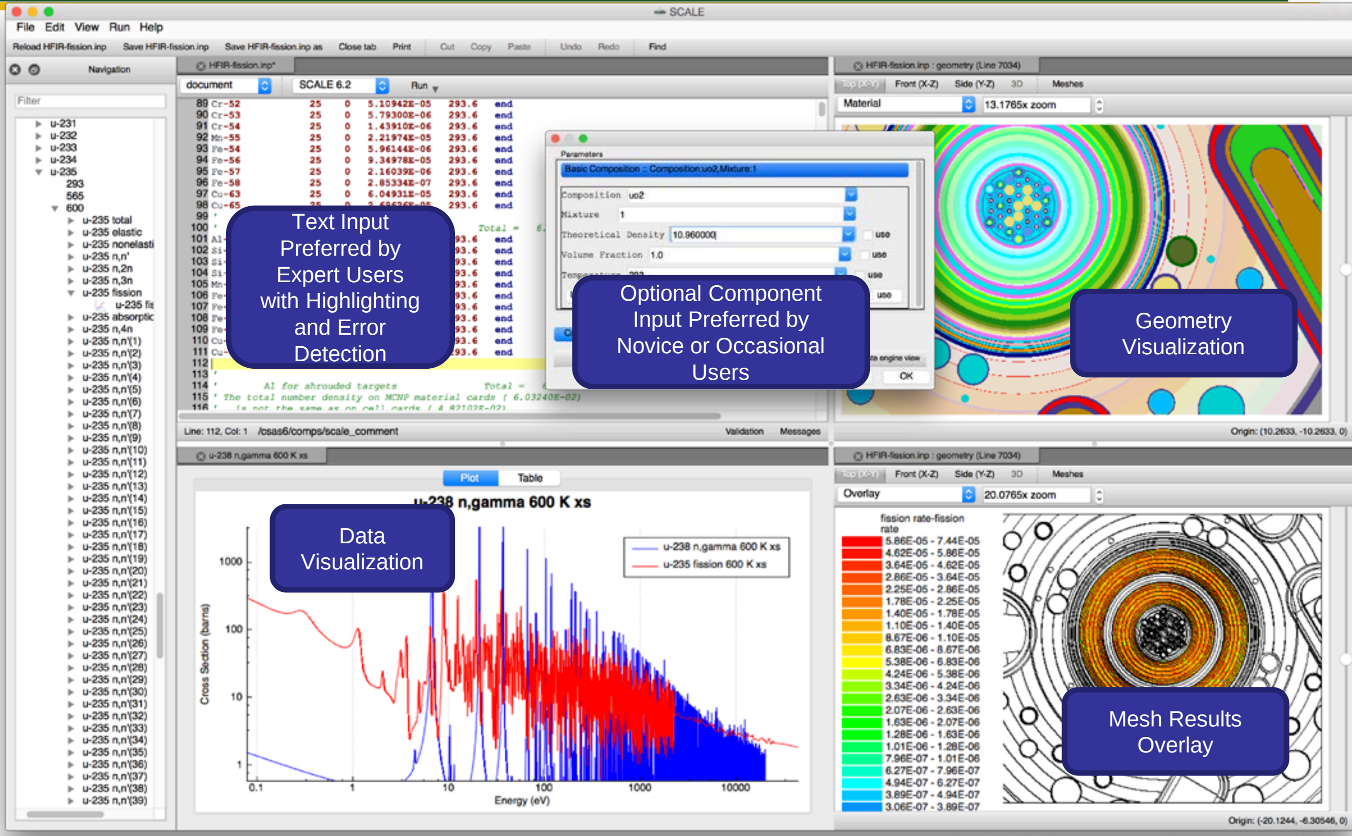
PROTEUS

Credit: TK Kim and Nicolas Stauff, ANL

NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

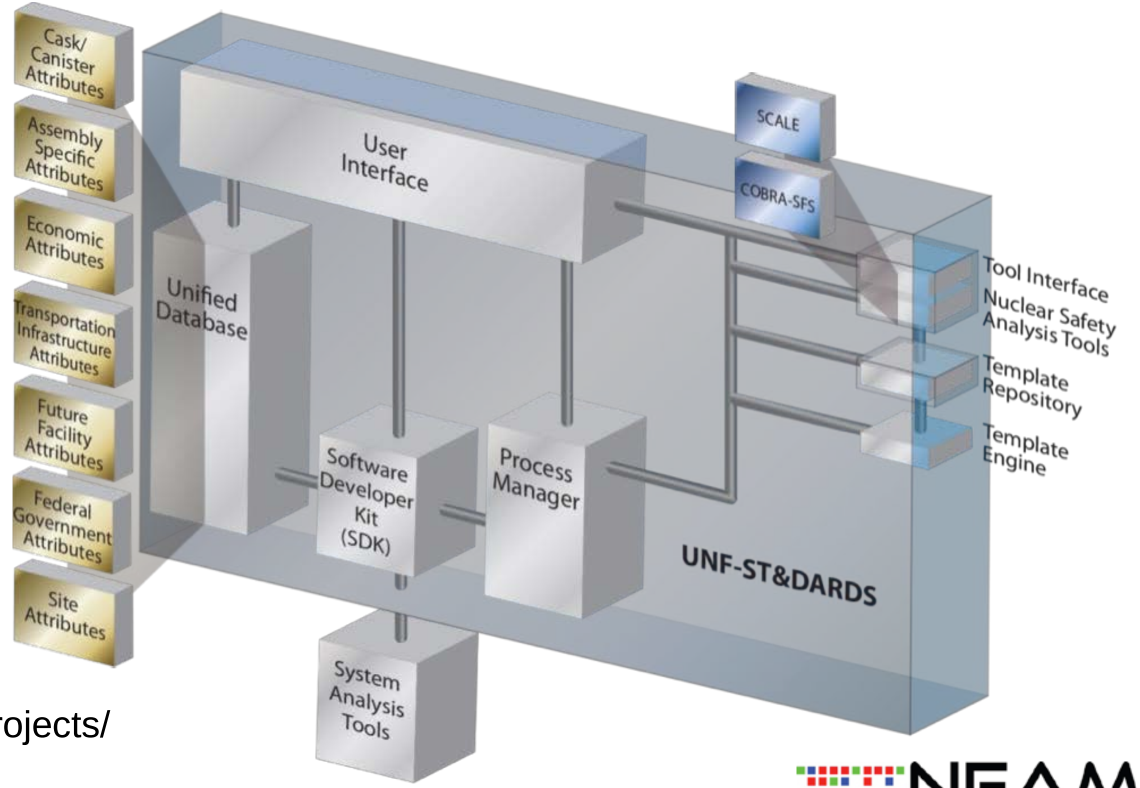
Fulcrum User Interface from SCALE

- **Debut release with SCALE 6.2 in April 2016**
  - 1700 licenses issued in first 9 months
- **Builds on 40-years of SCALE development experience**
- **Integrates capabilities of 8 independent interfaces from 2011 SCALE release**



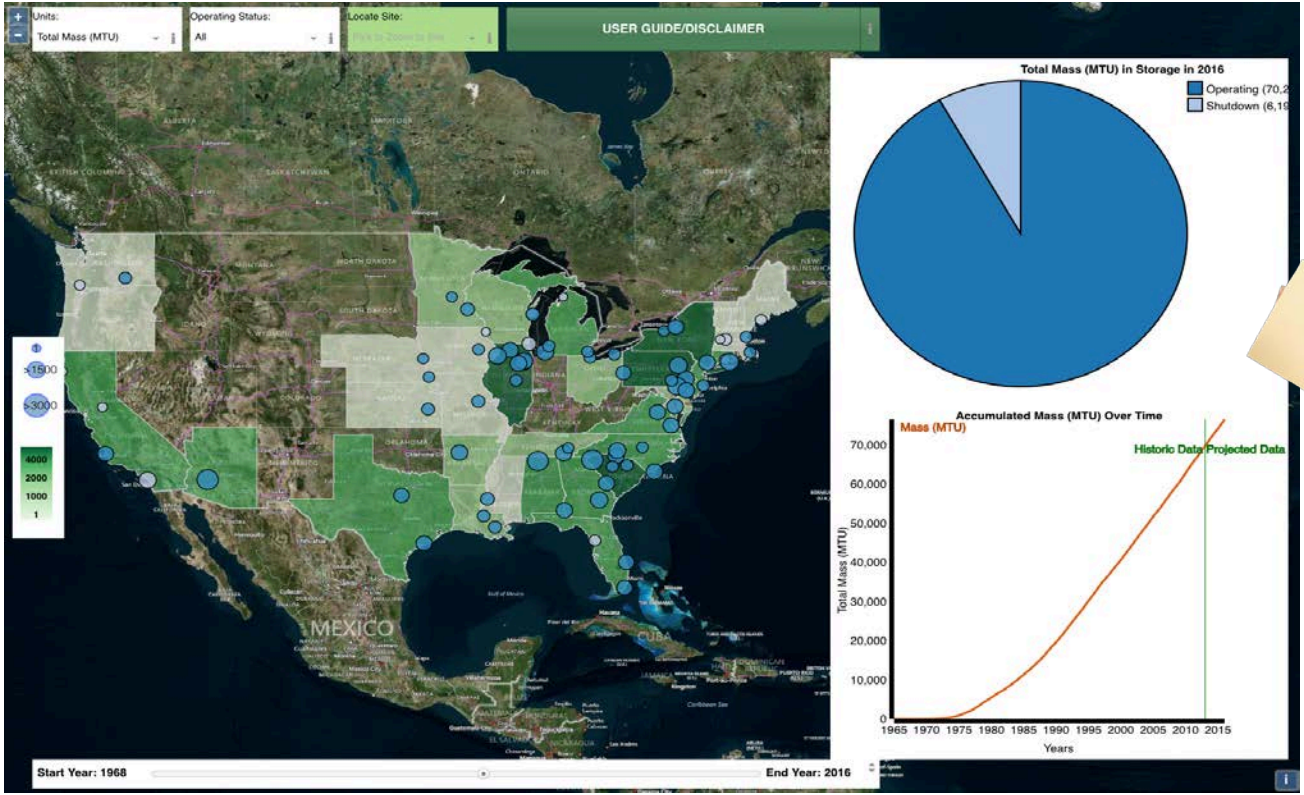
Used Nuclear Fuel-Storage, Transportation & Disposal Analysis Resource and Data System – UNF-ST&DARDS

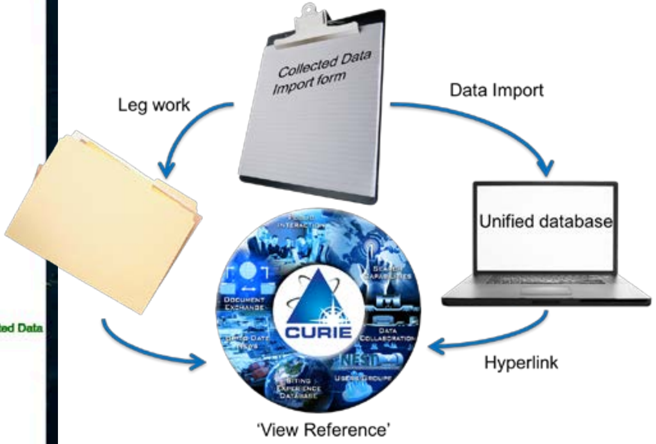
- **Developed for DOE-NE Nuclear Fuel Storage and Transportation Planning Project**
- **Unified Database consolidates key information from multiple sources and preserves data**
- **In use by NRC for licensing reviews**



https://www.ornl.gov/division/rnsd/projects/spent-nuclear-fuel-characterization

Goal: Generate as-loaded thermal, shielding, and criticality analysis for ~75,000 fuel assemblies in ~2,000 UNF canisters at 67 sites





http://curie.ornl.gov

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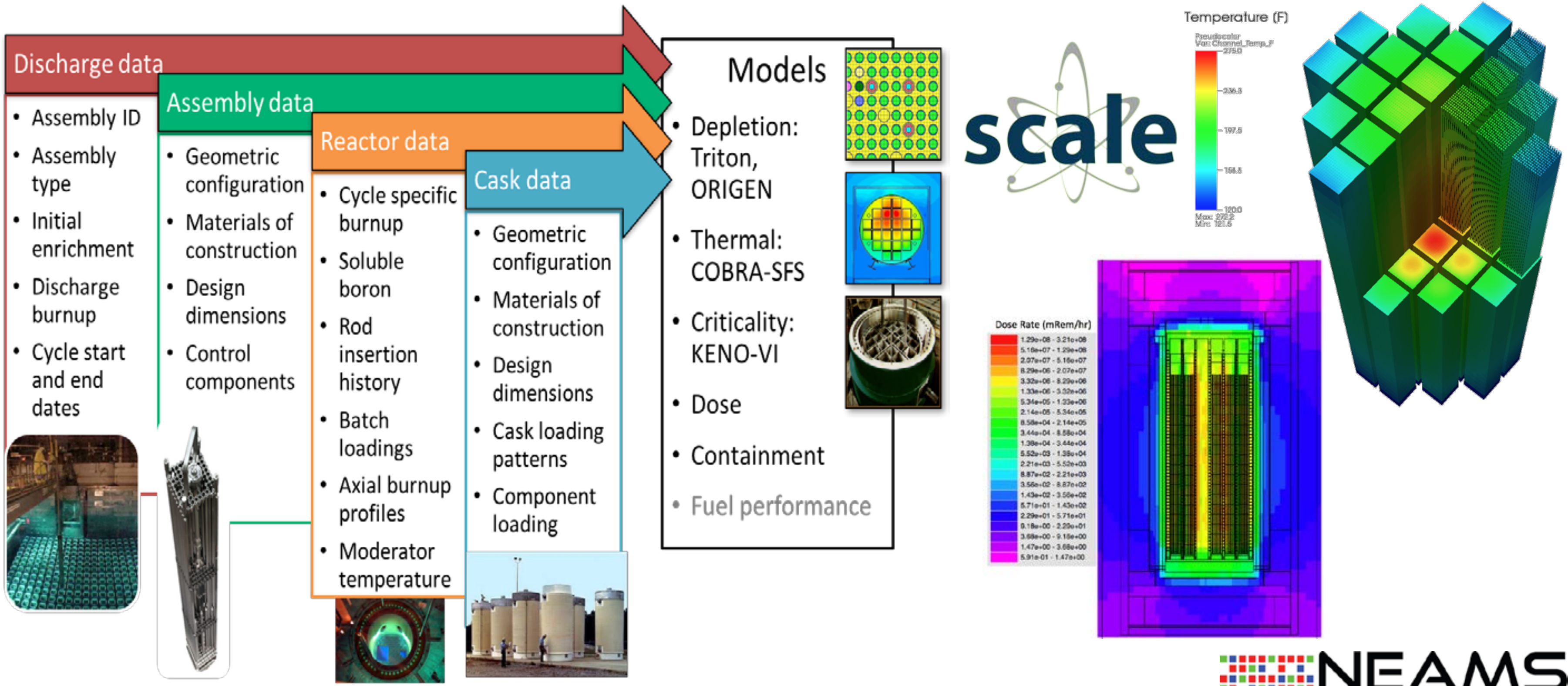
UNF-ST&DARDS integrates data with analysis capabilities to simplify UNF characterization process



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Nuclear Energy

NEAMS Workbench

Tool Integration for Advanced Nuclear Systems Analysis

Workflow Manager Guides Physics and Data Exchanges

User Selects Desired Fidelity of Physics

User Interface: Input Generation, Job Launch, Output Review, Visualization

System Templates and Workflow Manager

Cross Section Preparation	Neutronics	Depletion / Source Terms	Thermal Hydraulics / Plant Systems	Fuel Performance	Structural Analysis	Uncertainty Quantification
SCALE / XSProc	DIF3D	REBUS	SAS4A / SASSYS	LIFE-METAL	NUBOW	PERSENT
MC^2-3	PARCS	ORIGEN 2.2	SE2-ANL	PARFUME	DIABLO	Sampler
	MPact	ORIGEN	RELAP-5	BISON		Dakota
	Proteus		TRACE	MARMOT		
	MCNP		SAM			
	Shift		RELAP-7			
			NEK5000			

Production Tools

- NEAMS
- CASL
- Other

NEAMS

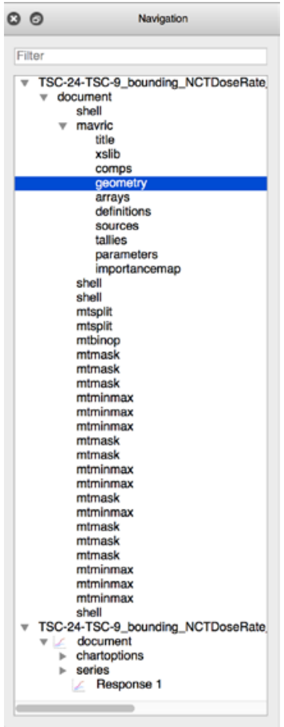
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

NEAMS Workbench Interface

Goal: Provide a cross-platform graphical user interface (GUI) designed to facilitate problem creation, modification, navigation, validation, and visualization, as well as output and data file interaction as needed by new and experienced users.

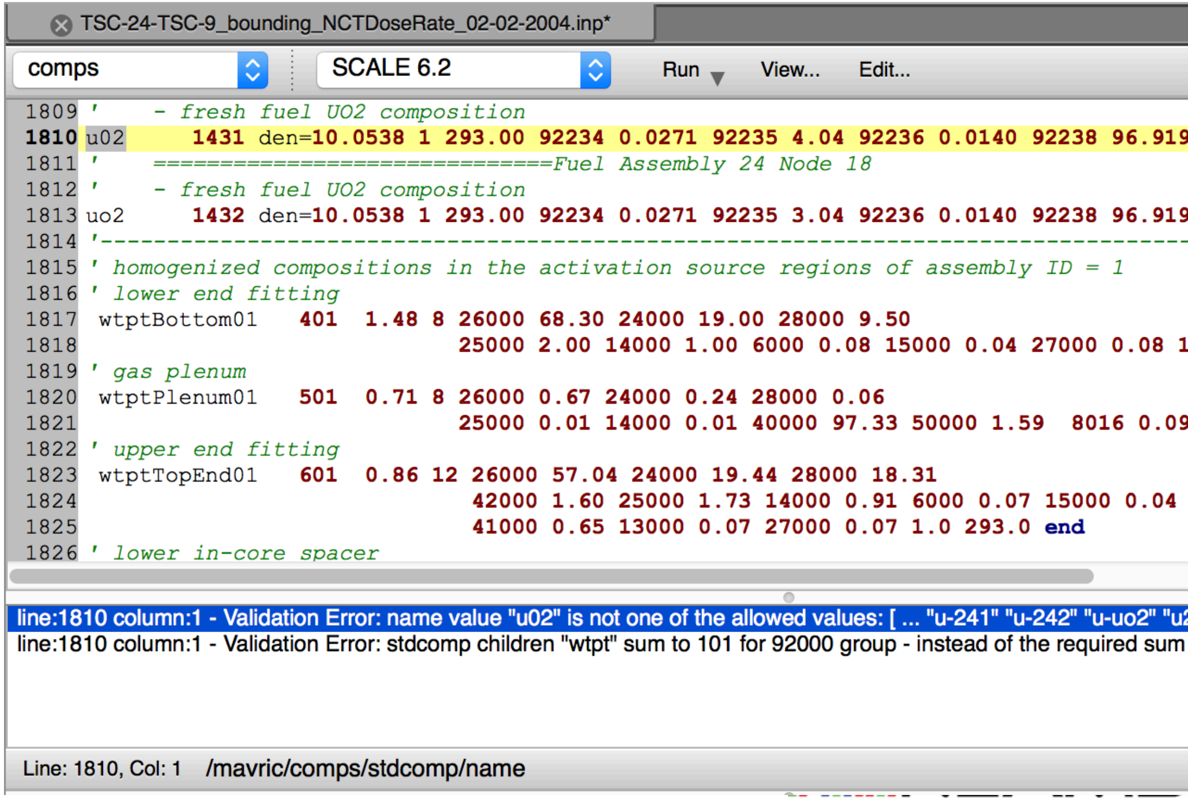
Document Navigation for Many Files

- **Hierarchical Listing of Document**
  - Quick Navigation to input component
  - Plot creation
- **Open Associated Files**
  - List files associated
  - Allows quickly opening associated files
- **Filter**
  - Regular expression based item filtering
- **Dockable**
  - Dock to main Fulcrum application
  - Float in separate window
  - Hide completely



Input Editor

- Syntax Highlighting
- Top Level Quick Navigation
- Cursor Context
- Preserves User Input Format
- Current Input Block Highlight
- Input Autocompletion
- Input Validation
- Customizable Input Execution



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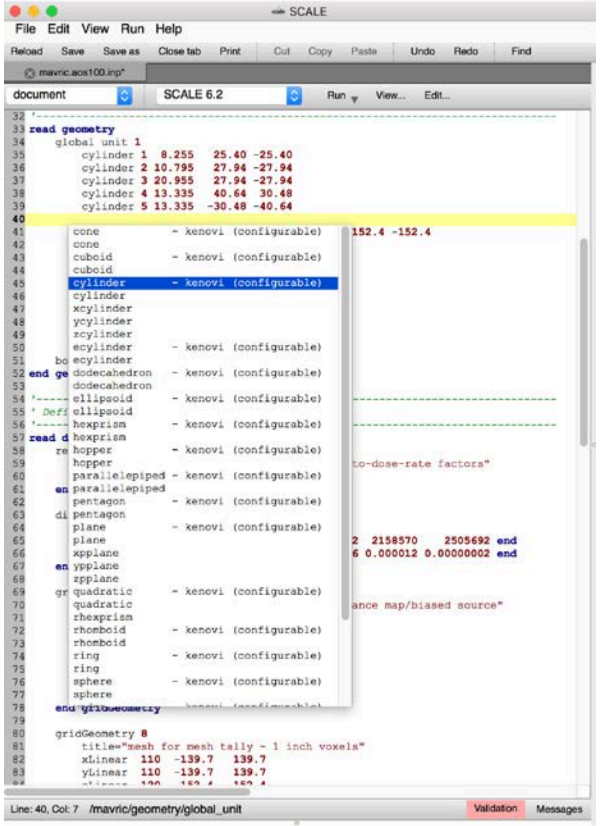
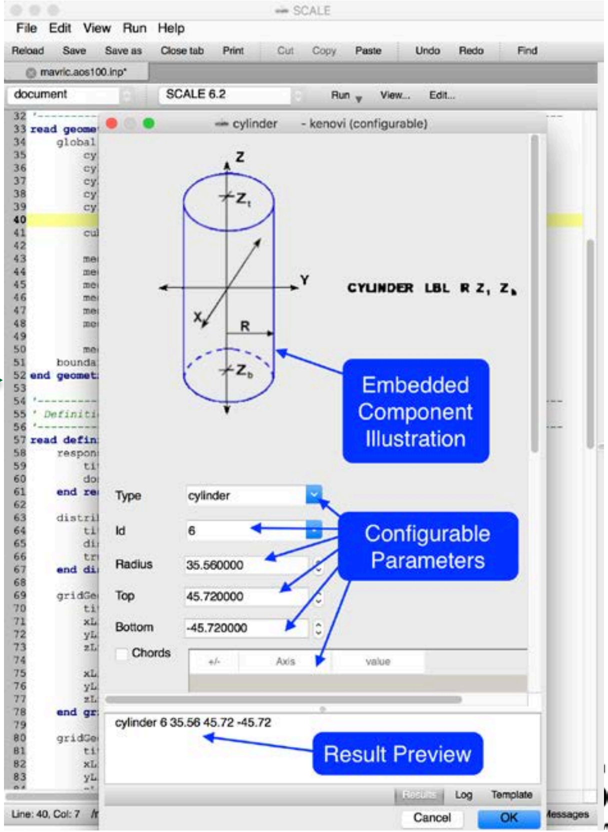
Input Autocompletion : Configurable Text

- List of available input options in context of current position in input file
- Optional input forms allow user to configure values prior to inserting into input.





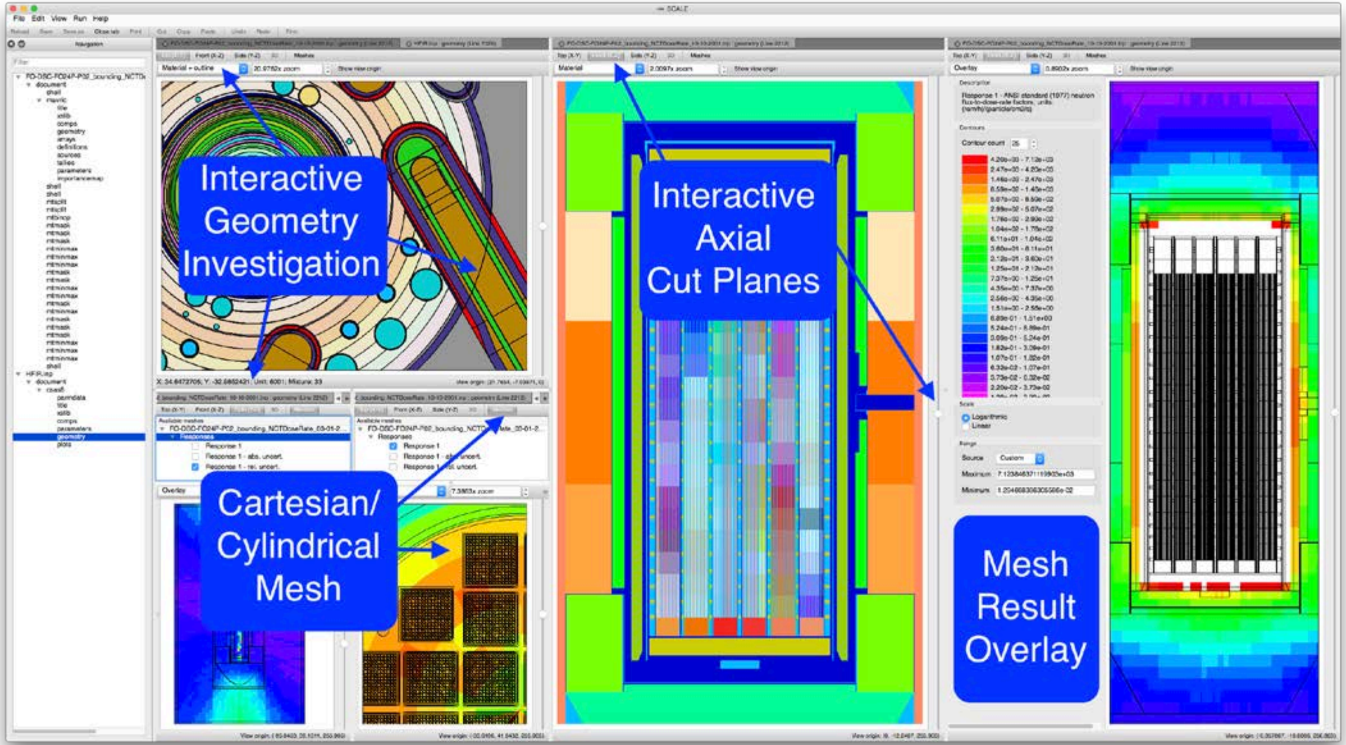
Access Autocomplete via
* CTRL+SPACE Keys, or,
* Edit…>Autocomplete

Data Plotting
(examples from SCALE)

- Supports most major SCALE data formats
- Will be extended to binary and ASCII formats for other codes
- Interactive and customizable
- Exports to image formats

Geometry Visualization
(examples from SCALE)

- Interactive and customizable
- Support for rapid geometry navigation and results overlay
- Integrating 3D visualization



Templated Common Input for Use with Many Codes

Engineering-style problem specific input
(type of system, materials, dimensions, timesteps, etc)

Database of supported system configurations
- Known systems and customizable features
- Input requirements and options for each code
- Code and problem specific information (mesh geometry, etc.)

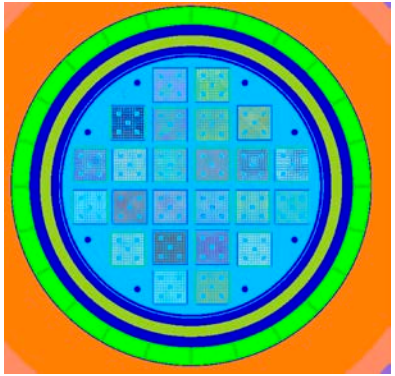
Template Engine Expansion

Input for Code A

Input for Code B

Input for Code C

Similar to CASL VERA-IN concept; Leverages Template Engine used for UNF-ST&DARDS and SCALE



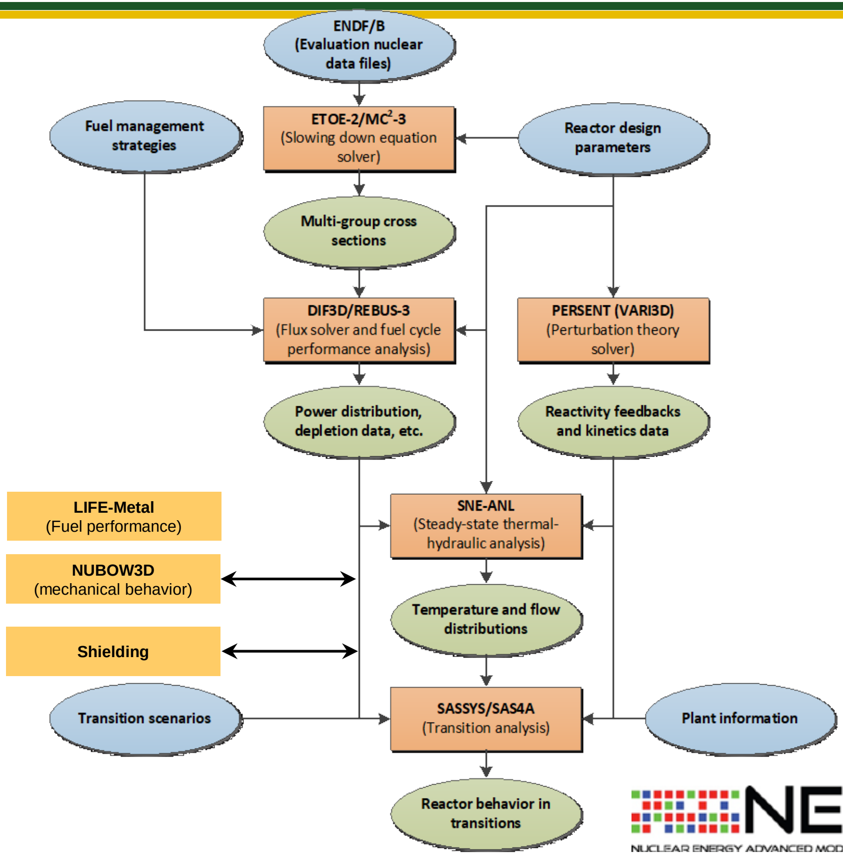
Workbench Integration of Legacy Codes: Advanced Reactor Codes (ARC)

- **ARC suite of codes developed with >30 years of experience:**
  - Highly efficient
  - Good accuracy (validated)

- **Different codes use:**
  - Similar design information
  - Different input logic

- **Scripts were developed by users to assist with input generation**

➢ **Difficult for new users to get started**
➢ **Limited user community**



Credit: Nicolas Stauff, ANL

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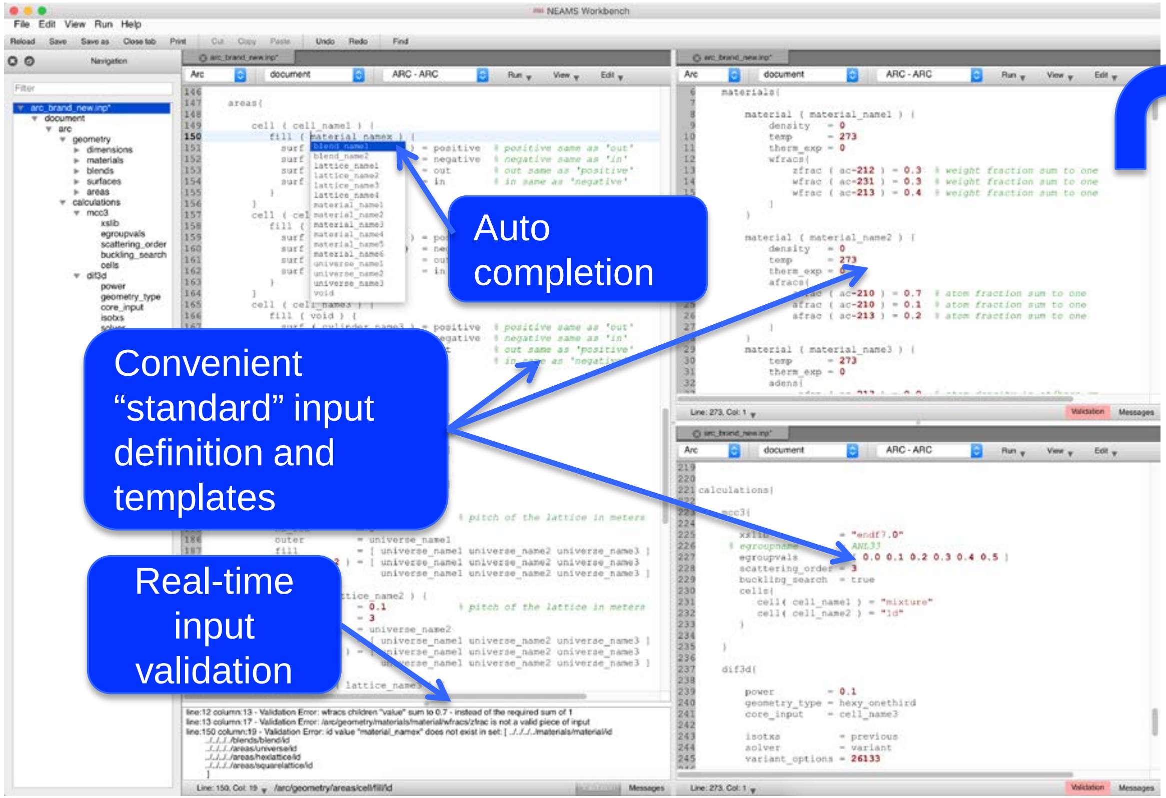
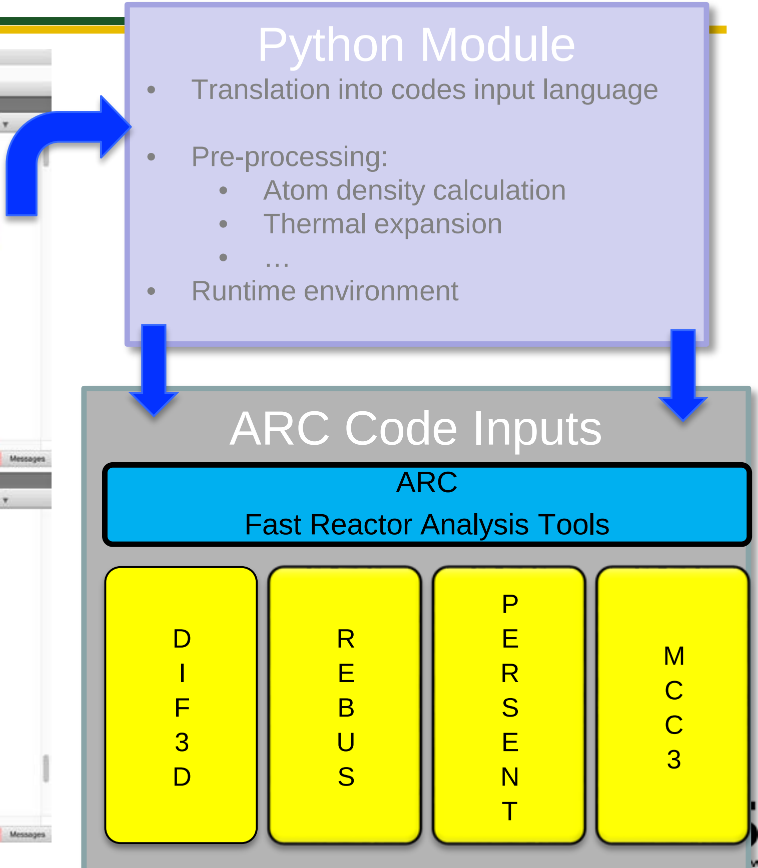
Approach to ARC/Workbench Integration





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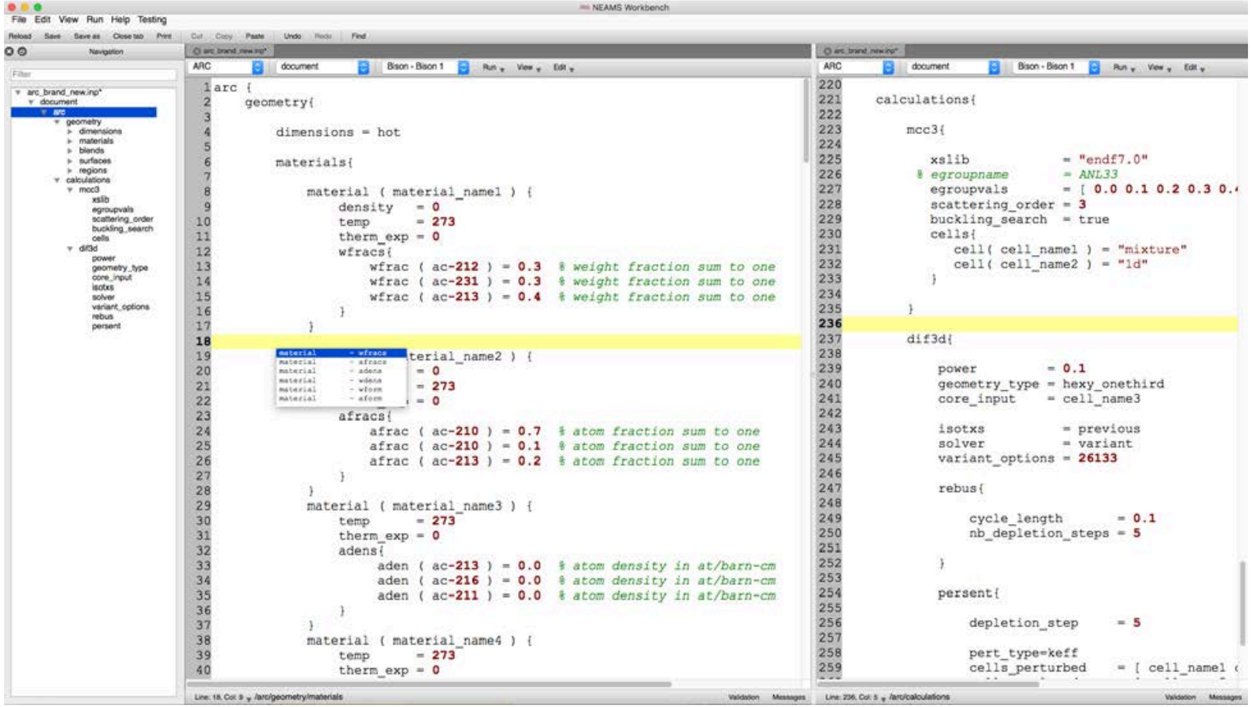
ARC/Workbench Input Definition

- **Convenient input structure based on MCNP logic:**
  - Well known logic
  - Very flexible and compatible with a wide range of other codes (PROTEUS, MCNP, *etc.*)
- **Developed in close collaboration with:**
  - ARC code system users
  - Code developers
- **Challenges:**
  - Keep input simple/attractive while compatible with deterministic codes' specific options
  - Interpret complex models and translate for lower fidelity code inputs



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BISON/Workbench Integration

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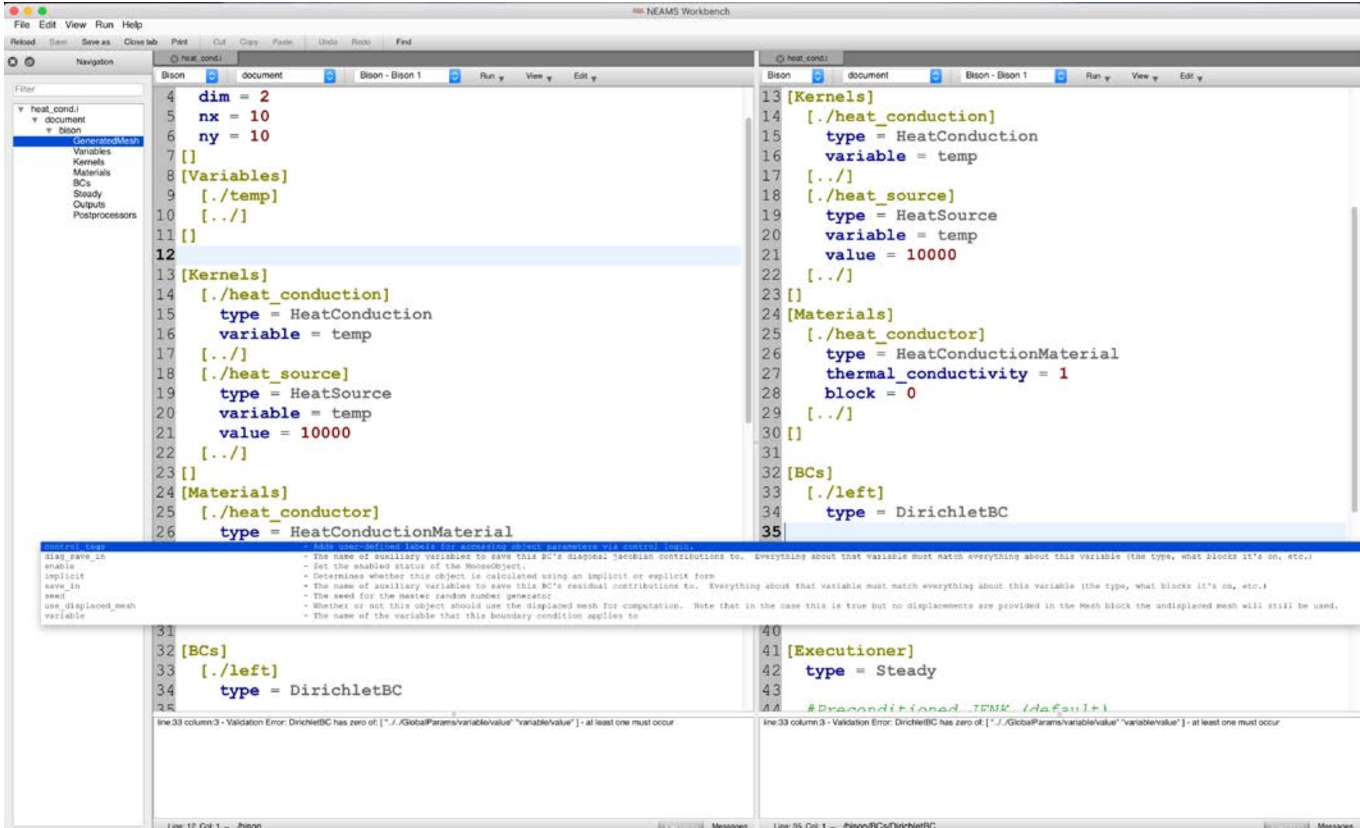
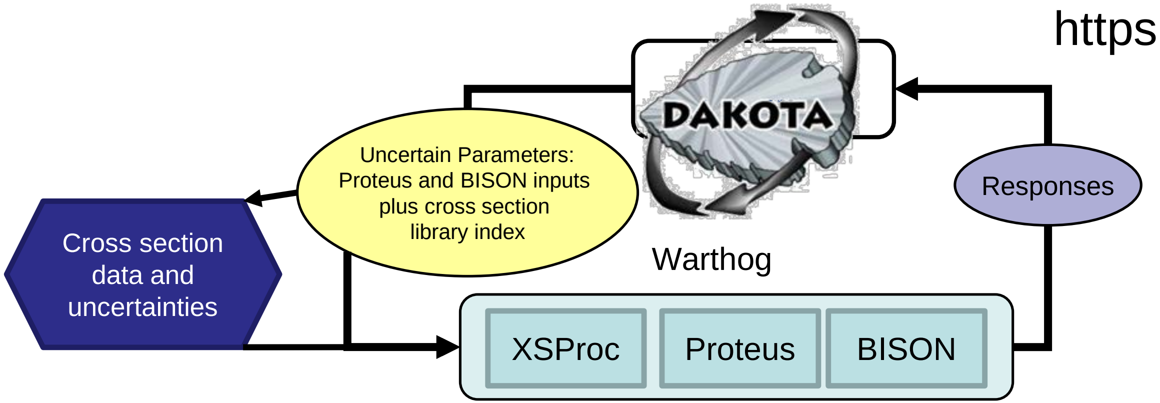
- MOOSE applications easily enabled under Workbench with uniform input standards available through MOOSE
- Runtime updated to execute BISON
- MOOSE's input module is being updated to generate files needed by Workbench, even for new applications generated by external teams



Dakota: Suite of iterative mathematical and statistical methods that interface to computational models

- **Algorithms for design exploration and simulation credibility**
- **Makes sophisticated parametric exploration of simulations practical for a computational design-analyze-test cycle**
- **Provides scientists and engineers (analysts, designers, decision makers) greater perspective on model predictions:**
  - Enhances understanding of risk by quantifying margins/uncertainties
  - Improves products through simulation-based design, calibration
  - Assesses simulation credibility through verification and validation

https://dakota.sandia.gov/



Workbench Installation Process

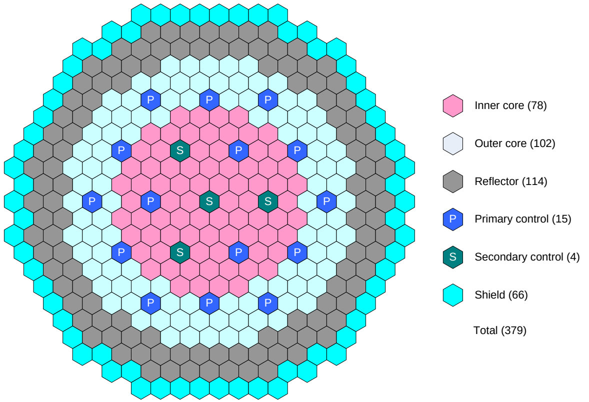
- **Mac:**
  - Download disk image and expand
  - Drag and drop
- **Windows:**
  - Download installer and expand
  - Double-click, follow instructions
- **Linux**
  - Download tarball
  - Unpack

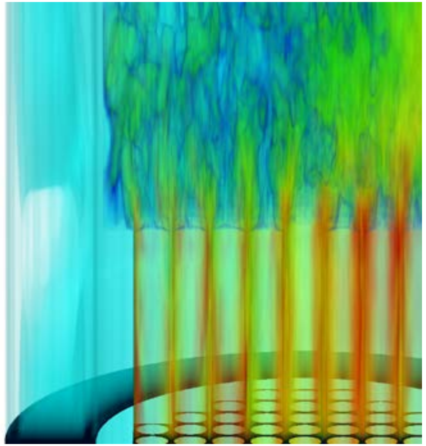
- **Must also license, obtain, install, configure, build computational tools that will be called from Workbench**

Current NEAMS Workbench Activities

- **Tool integration**
  - NEAMS Tools –
    - INL - MOOSE, BISON
    - ANL - MC^2-3, PERSENT, NEK5000
    - SNL – Dakota
    - ORNL - Warthog
  - Current Production Tools –
    - ORNL – SCALE 6.2
    - ANL - DIF3D, REBUS
- **Capabilities**
  - Visualization –
    - LBNL – VisIt
    - Kitware – Paraview, VTK
  - Customized configurations
  - Job launch/queuing tools

- **Application Templates**
  - WPRS SFR-UAM Sodium fast reactor benchmark
  - WPRS UAM-LWR fuel performance benchmark w/ UQ





Workbench NEAMS Planned Activities

- **Add support for additional codes (esp. NEAMS codes) and templates of openly available systems**
- **Training opportunity for initial users/code integrators**
  - ORNL June 2017
- **Current Deployment**
  - Fulcrum available with SCALE 6.2; can issue Workbench alpha version for testing w/ SCALE license
  - Deploy beta version to RSICC in September 2017
  - Moving to open source to separate from SCALE and facilitate real-time collaboration with many teams
- **Future Development**
  - High-to-Low fidelity capabilities with some proposed approaches:
    - Machine learning
    - Surrogate models
    - Bayesian techniques
    - Other?
  - Mesh geometry for common systems
  - Tools to facilitate/automate mesh generation (integrate commercial tools?)

NEAMS Initiatives

- Develop, apply, deploy, and support state-of-the-art predictive modeling and simulation tools for the design and analysis of current and future nuclear energy systems using computing architectures from laptops to leadership class facilities
- Engage industry and regulators through GAIN to provide computational tools for advanced reactors and advanced fuels
- Integrate many tools for industry and regulatory use through the NEAMS Workbench

A Multiscale FHR Modeling and Simulation Approach Employing NEAMS Tools

Rich Martineau (INL)

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A Multiscale, Multiphysics FHR Modeling and Simulation Approach Employing NEAMS Tools

Richard C. Martineau
Idaho National Laboratory

March 8, 2017

Workshop on Tools for Modeling and Simulation of Fluoride Cooled High Temperature Reactors (FHR)

Georgia Institute of Technology, Atlanta, Georgia

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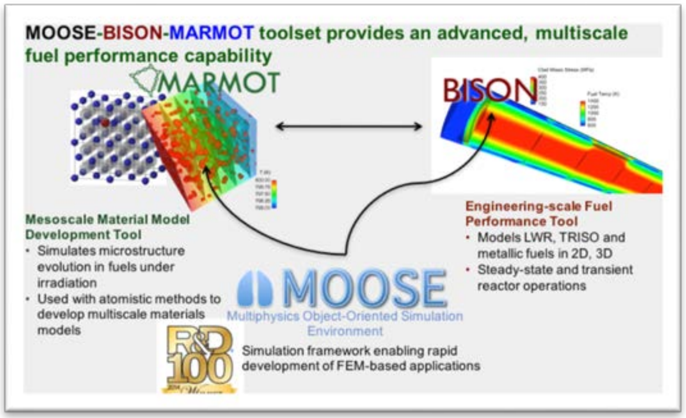
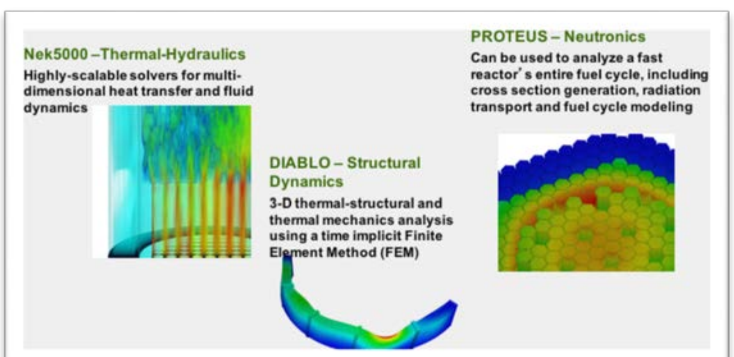
NEAMS (Nuclear Energy Advanced Modeling and Simulation) Program

Aim: Develop, apply, deploy, and support a predictive modeling and simulation toolkit for the design and analysis of current and future nuclear energy systems using computing architectures from laptops to leadership class facilities.

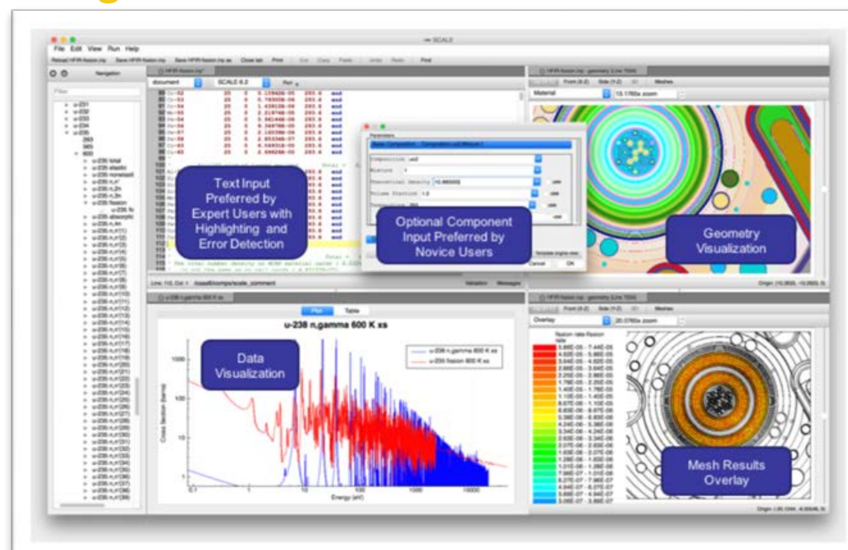
Fuels Product Line



Reactor Product Line



Integration Product Line



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A multiscale, multiphysics FHR modeling and simulation approach employing NEAMS tools (well mostly)

- **The Fluoride-salt-cooled, high-temperature reactor (FHR) integrates a high-temperature, low-pressure liquid salt coolant, with a high-temperature coated-particle fuel, and a Brayton power cycle, all in a passively safe pool-type reactor design.**

- **There are three obvious length scales associated with FHRs:**
  - *Lower Length Scale (LLS), less than 0.5 meter*
  - *Engineering Length Scale (ELS), reactor vessel length*
  - *Reactor Plant Scale (RPS), 10s of meters*

- **Integrating multiple length (and time) scales requires framework flexibility, i.e., the ability to pass information up and/or down the scales in a tightly-coupled fashion.**

- ***The NEAMS MOOSE framework is flexible!***

MOOSE: NEAMS Multiphysics Computing Framework

- ***MOOSE:* (Multiphysics Object-Oriented Simulation Environment)**
  - INL/ANL HPC multiphysics software development & runtime framework.
  - Started in May of 2008 (LDRD).
  - Subjected to multiple peer-reviews, NQA-1 compliant.

- *MOOSE* is an C++ object-oriented software framework allowing rapid development of new simulation tools.
- 1D, 2D or 3D FEM (CG, DG and XFEM) with both mesh and time step adaptivity.
- Application development focuses on implementing physics (PDEs) rather than numerical implementation issues.
- Leverages multiple DOE and university developed scientific computational tools (MPI, PETSc, LibMesh, Hypre, etc.).
- Seamlessly couples native (MOOSE) applications using *MOOSE MultiApps and Transfers.*
- Efficiently couples non-native (and non-C++) codes using *MOOSE-Wrapped Apps.*
- Obtained Free Software Foundation, Inc.'s Lesser General Public License Version 2.1on February 12, 2014. *MOOSE* also received a 2014 R&D 100 Award.

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Lower Length Scale Approach

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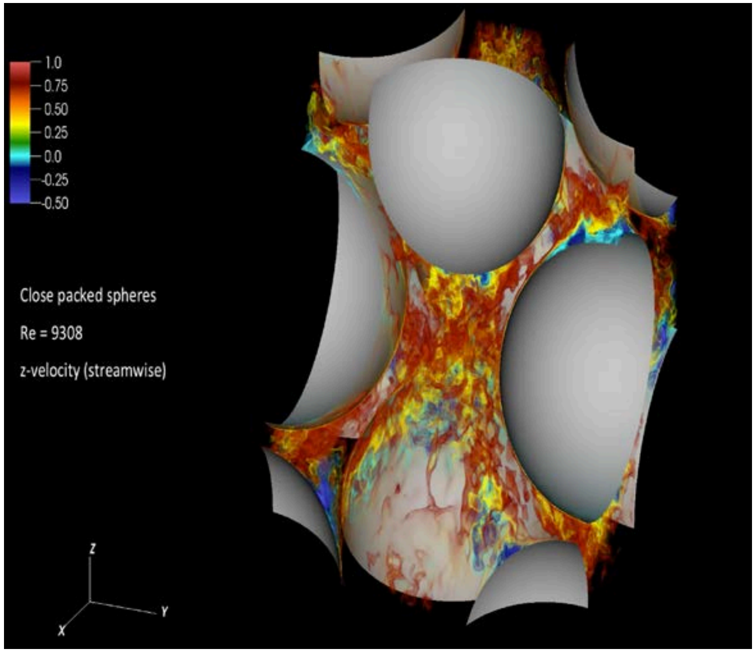
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

FHR Lower Length Scale (LLS) Approach

The FHR LLS will focus upon resolving the high-resolution physics associated with detailed reactor physics (radiation transport), highly turbulent conjugate heat transfer (CHT) with highly resolved thermal BLs (heat flux), and multi-scale TRISO nuclear fuels performance.

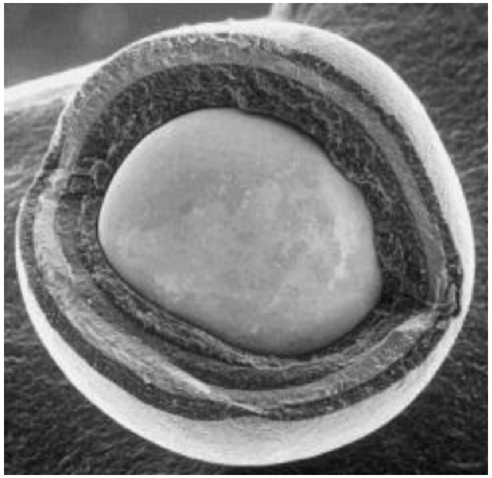
NEAMS LLS Applications:

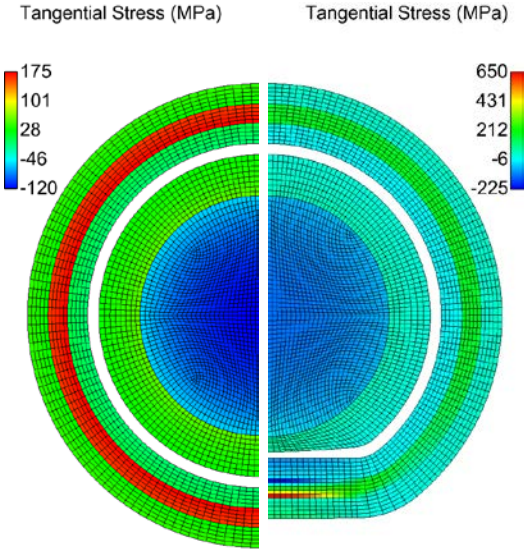
- ***Nek5000*** **is an open source highly-scalable CFD solver (https://github.com/Nek5000) and the NEAMS toolkit's high-resolution, multi-dimensional thermal fluids module. *Nek5000* is being developed at Argonne and has been used in a variety simulations to gain unprecedented insight into the physics of turbulence in complex flows.**

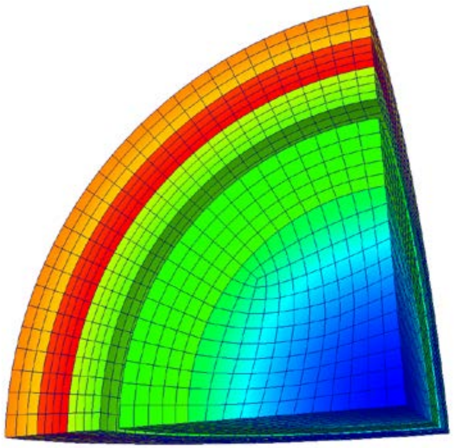


FHR LLS Approach (cont'd)

- ***BISON*** **(Broadly Implicit Simulation Of Nuclear fuels) is designed to be an "all-nuclear fuel" simulation capability, including current LWR fuels, next generation accident tolerant fuels, TRISO fuels, plate fuels, fast oxide and metal fuels, etc.** ***BISON*** **is coupled to the NEAMS** ***Marmot*** **microstructure fuels application, which predicts coevolution of the microstructure and physical properties to correct** ***BISON's*** **empirical models.** ***BISON/Marmot*** **provides for NEAMS multiscale fuels performance capability.**
  - *BISON* TRISO fuel capabilities already exist in 1D, 2D, and 3D

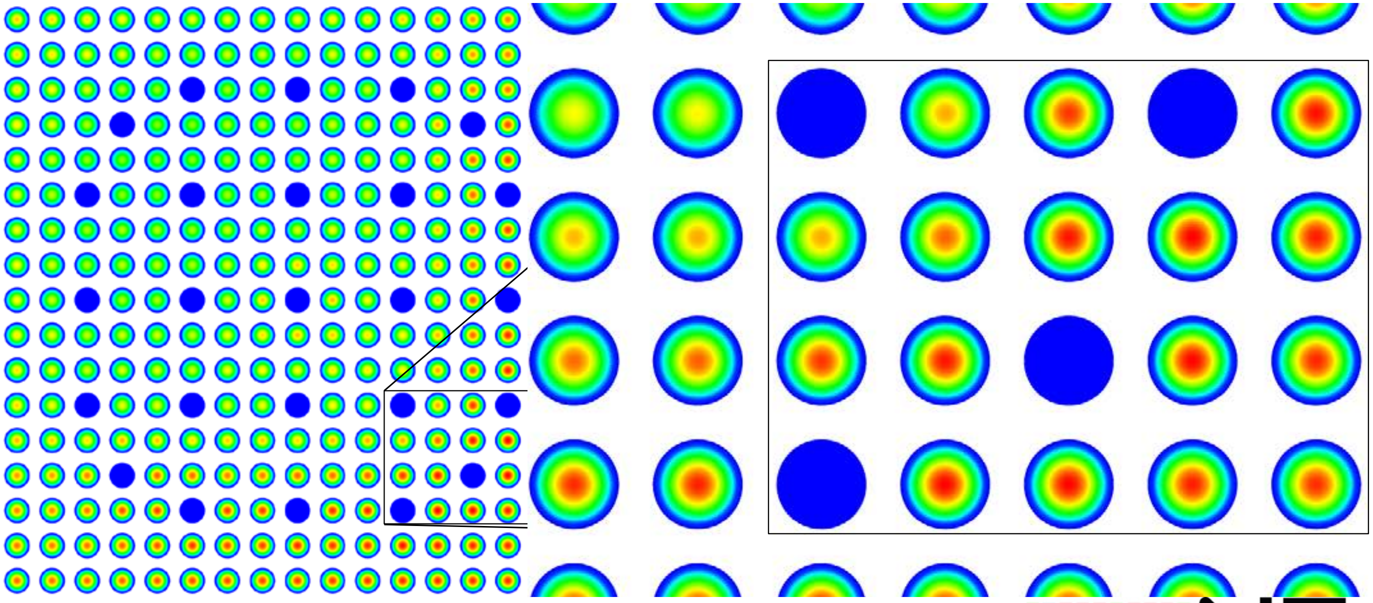






FHR LLS Approach (cont'd)

- *OpenMC* is an open source Monte Carlo particle transport simulation code (https://mit-crpg.github.io/openmc/), developed at MIT and Argonne. It is capable of simulating 3D models based on constructive solid geometry with second-order surfaces. The particle interaction data is based on ACE format cross sections, also used in the MCNP and Serpent Monte Carlo codes.

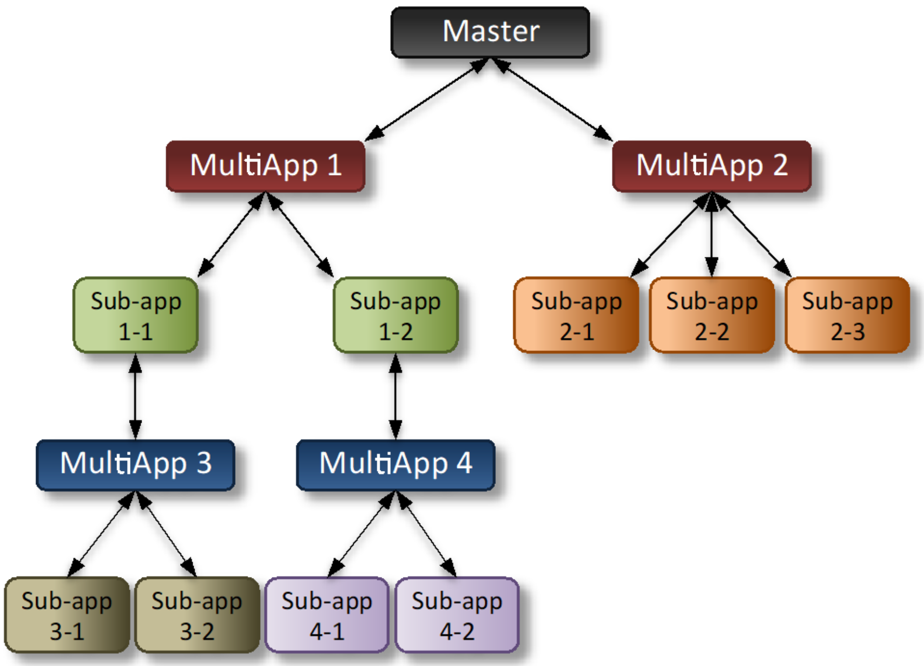


BISON heat conduction solution

FHR LLS Approach (cont'd)

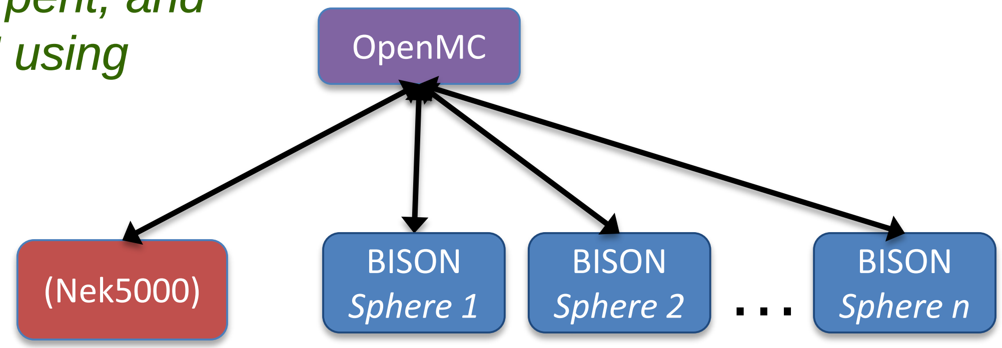
- **MOOSE was originally created to solve fully-coupled systems of PDEs.**
- **Not all multiphysics systems need to be / are fully coupled:**
  - Systems with multiple space and/or timescales.
- **The MultiApp system allows multiple MOOSE (or external) applications to run simultaneously in parallel.**
  - A single MultiApp might represent thousands of individual solves.
- **The Transfer system in MOOSE is designed to push and pull fields and data to and from MultiApps.**
- **The MOOSE MultiApps and Transfers system has been efficiently adapted for non-native applications called "MOOSE-Wrapped Apps"**
  - OpenMC, Serpent and Nek5000 so far.

Tightly-coupled multiphysics using MOOSE

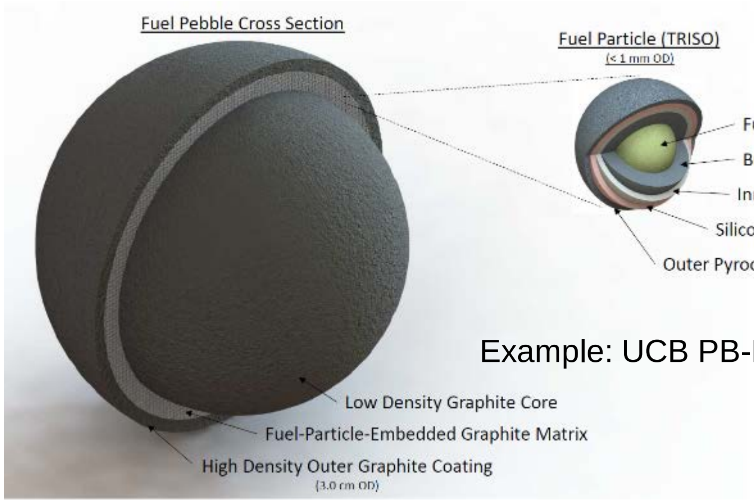


FHR LLS Approach (cont'd)

Within the last year, both Nek5000, Serpent, and OpenMC have been coupled to BISON using MOOSE-Wrapped Apps.



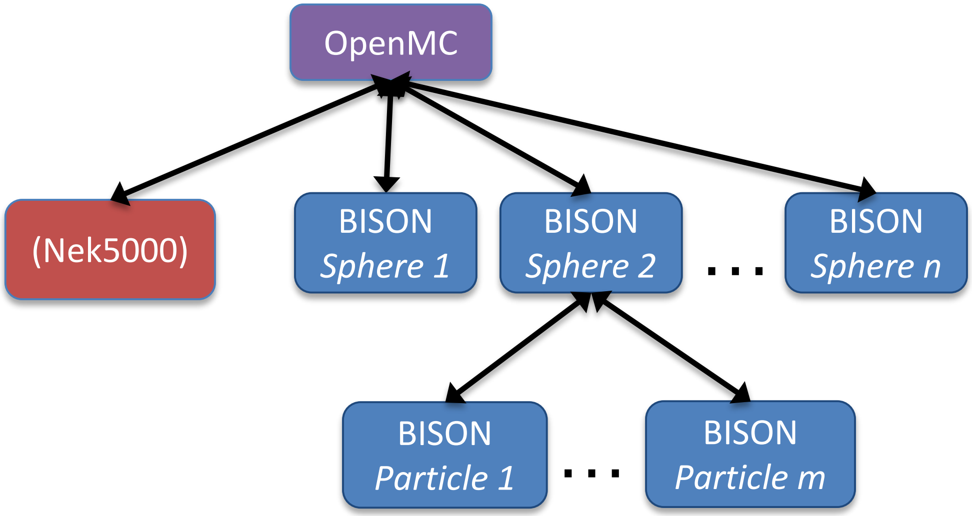
- **Arbitrarily choose OpenMC as the "MasterApp". Only one instance needed as the radiation field is continuous across the domain.**
- **Let *Nek5000* be one of the "MultiApps. Again, only one instance is needed.**
- **Let *BISON* also be a MultiApp representing homogenized fuel pebbles (spheres). A typical LLS calculation might involve twenty pebbles (*n=20*), or twenty instances of *BISON* MultiApps.**
- ***BISON* MultiApps would be composed of homogenized fuel properties (graphite, SiC, UO_2).**

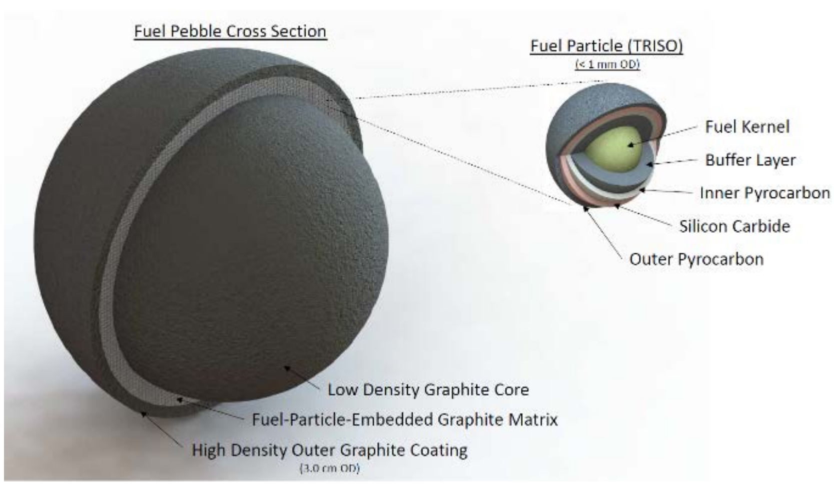


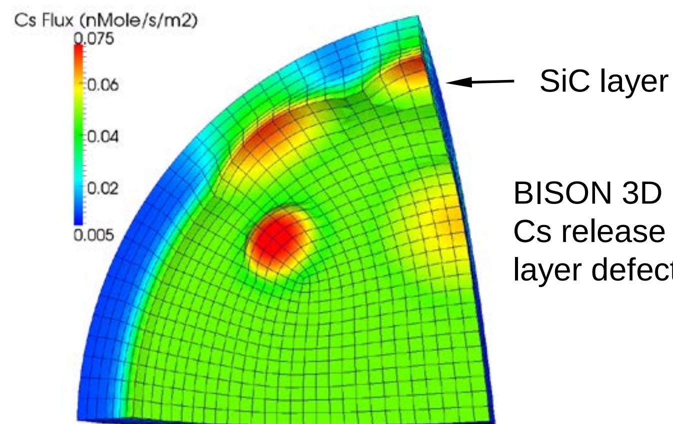
Example: UCB PB-FHR

FHR LLS Approach (cont'd)

- **If greater uncertainty is required in the fuel calculation, *BISON* could serve as it's own sub-millimeter lower length scale informed Sub-App by analyzing particle behavior on the homogenized sphere.**
- **As many instances, *m*, of *BISON* Sub-Apps may be initiated as necessary.**



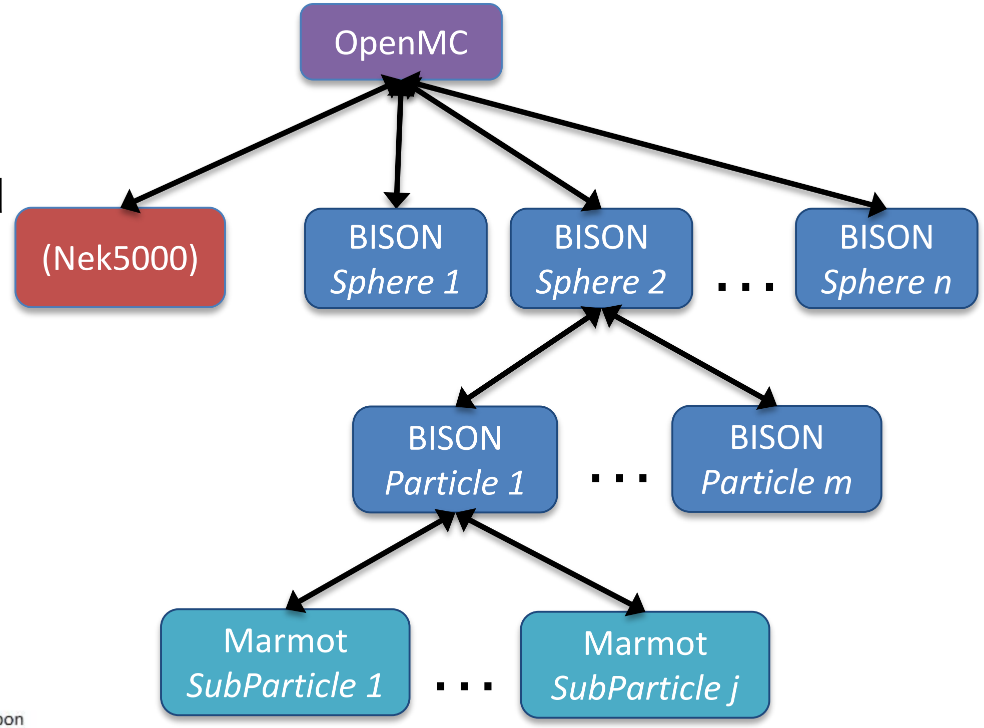


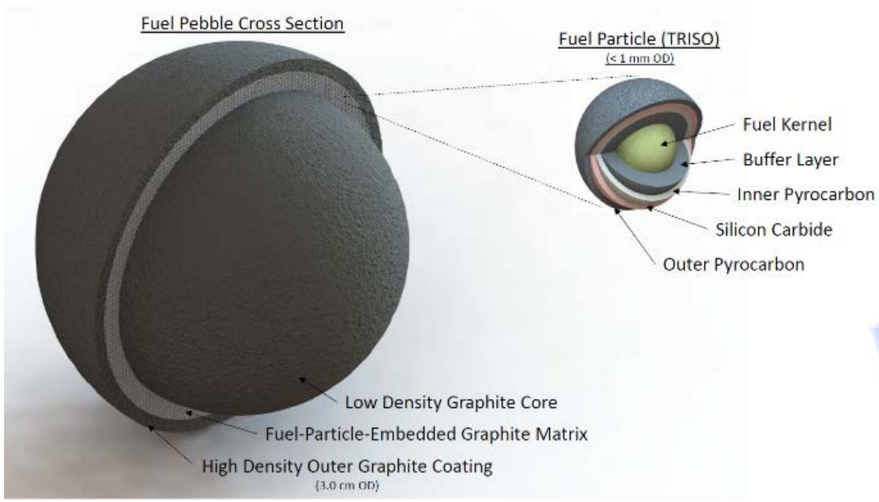


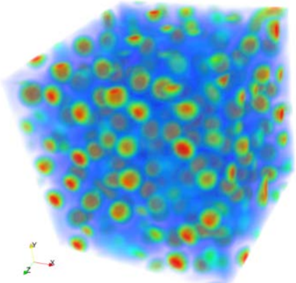
BISON 3D result for Cs release in SiC layer defects

FHR LLS Approach (cont'd)

- **If detailed FGR inventories or determination of fuel damage effects is required, *j* instances of Marmot Sub-Apps may be initialed in the fuel kernel or layers. *Convergence may be slow!***
- **Also good for SciDAC proposals and Gordon Bell Prize awards.**







Marmot fission gas bubble formation and migration in UO_2

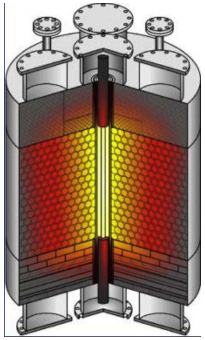
FHR LLS Approach (cont'd)

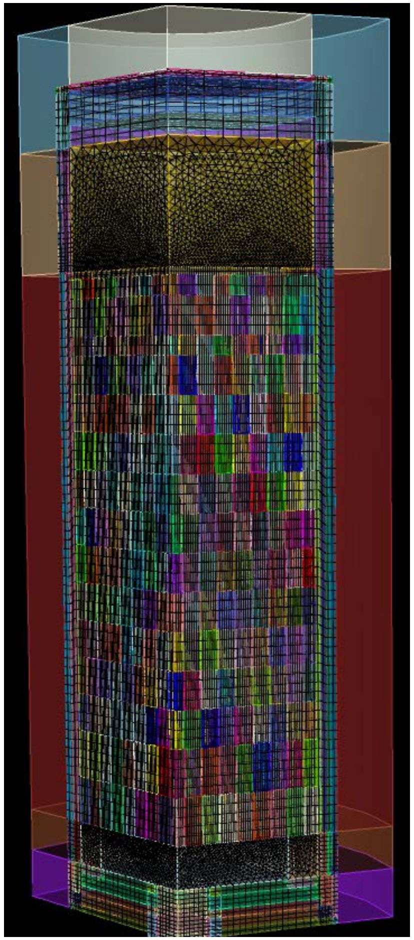
- **Over the years, I have heard industry repeatedly state that they don’t care about “high-resolution” physics calculations. They are only interested in “engineering” applications that run fast.**
- **However, LLS simulations provide for:**
  - High-resolution simulation of validation experiments can help optimize the experiments by providing insight as to where, what, and when to measure parameters. The resulting iterative process will yield a validated capability.
  - High-resolution simulations can cheaply provide closure relations for the “engineering” applications in the absence of detailed empirical data.
  - With a “science-based predictive capability,” the physics of off-normal behavior, such as in rapid reactivity events, may be analyzed in detail for failure mechanisms.
- **Under GAIN/NEAMS, DOE-NE is providing this LLS simulation capability, including access to high end hardware, for free.**

Engineering Length Scale Approach

FHR Engineering Length Scale (ELS) Approach

The FHR ELS will serve as an intermediate resolution of core physics, providing two- and three-dimensional full core calculations, albeit in a homogenized approach.





NEAMS ELS Applications:

- ***Pronghorn*** **is a multi-dimensional coarse mesh reactor simulator based upon the** ***MOOSE*** **framework. Pronghorn is designed for both cylindrical (*r-z*) and three-dimensional geometries. Pronghorn physics can be described as homogenized conjugate heat transfer (CHT), where each finite element may contain a mixture of coolant, fuel, moderator, or other core internals. Originally developed for VHTR (or HTGR) concepts (prismatic and pebble-bed), Pronghorn is currently under development at UCB as an FHR core simulator.**
- ***Pronghorn*** **has considerable pebble bed capability and is benchmarked against PBMR-400 and SANA for HTGR applications.**

Simple, Pebble-Bed Model for *Pronghorn*

***Think of the model as a two-phase flow problem where the second phase (pebble stack) is stationary*.**

Conservation of Mass

$$\frac{\partial \alpha\rho_g}{\partial t} + \vec{\nabla}\cdot\alpha\rho_g\vec{u}_g = 0$$

Assumptions:

1. No bed motion
2. No phase change
3. Ensemble-averaged turbulence effects

Balance of Momentum

$$\frac{\partial \alpha\rho_g\vec{u}_g}{\partial t} + \vec{\nabla}\cdot\left(\alpha\rho_g\vec{u}_g\otimes\vec{u}_g\right) = -\alpha\vec{\nabla}p_g - \xi\rho_g\left\|\vec{u}_g\right\|^2\vec{\nabla}\alpha - \lambda\vec{u}_g$$

Conservation of Energy

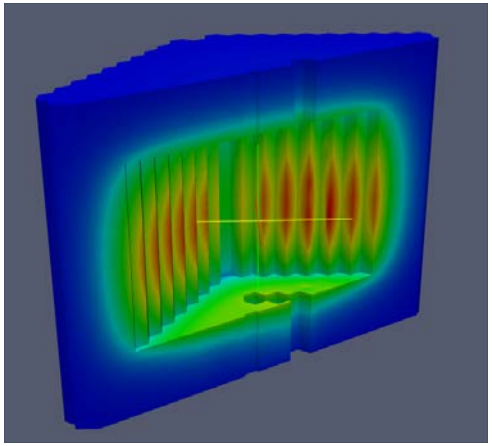
$$\frac{\partial\alpha\rho_g E_g}{\partial t} + \vec{\nabla}\cdot\left(\alpha\rho_g\vec{u}_g H_g\right) + \vec{\nabla}\cdot\alpha\vec{q}_g - \alpha\rho_g\varepsilon_g = \vartheta\left(T_s - T_g\right)$$

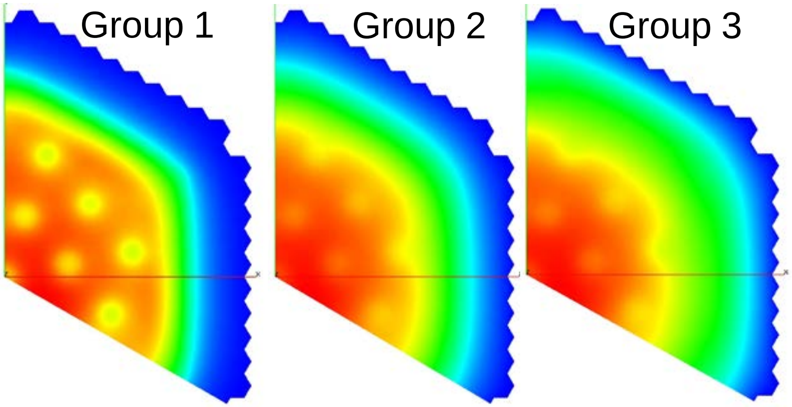
$$\frac{\partial\left(1-\alpha\right)\rho_s e_s}{\partial t} + \vec{\nabla}\cdot\left(1-\alpha\right)\vec{q}_s - \left(1-\alpha\right)\rho_s\varepsilon_s = -\vartheta\left(T_s - T_g\right)$$

Mk1 pebble core geometry showing fuel pebble (green) and graphite reflector pebble (yellow) regions.

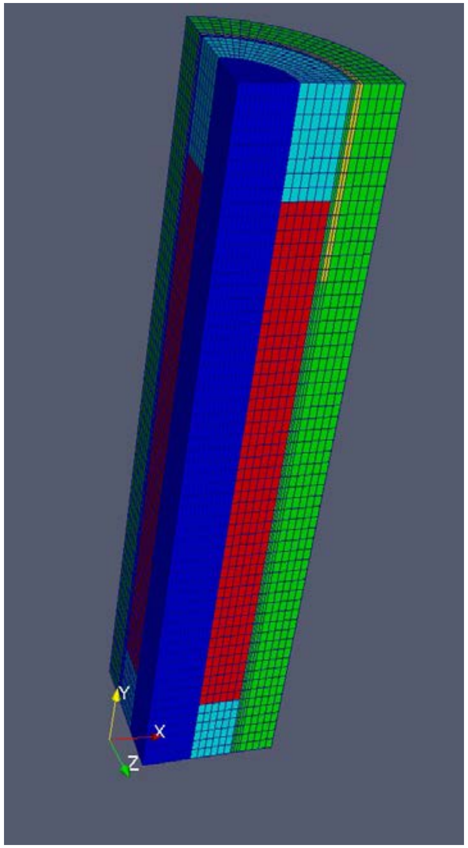
FHR ELS Approach (cont'd)

- ***Rattlesnake*** **is a *MOOSE*-based multi-level, multi-scale radiation transport application being developed for the TREAT simulator under a multi-year NEAMS work package at INL. Rattlesnake is capable of performing time dependent transport calculations with multiple transport schemes, including multi-group diffusion, spherical harmonics, and first- and second-order Sn.**
  - Multi-group diffusion is full-core pebble bed method of choice.





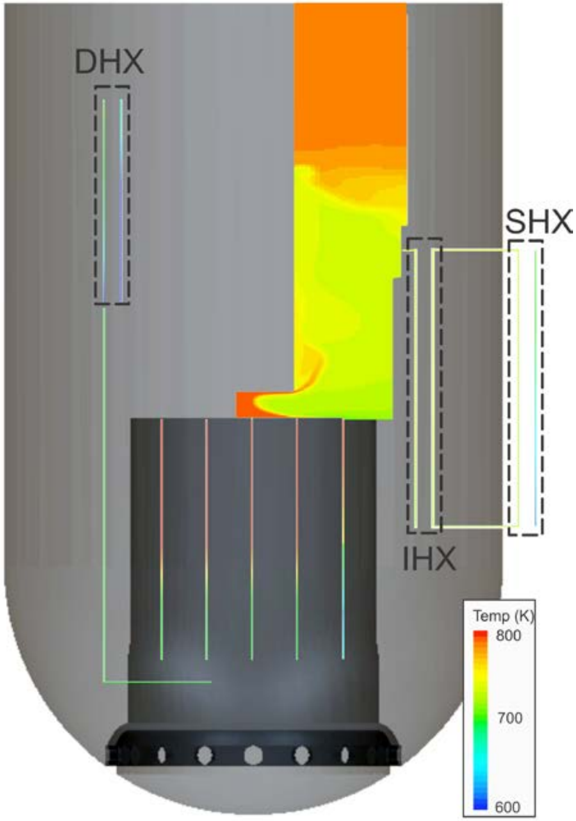
2D 3-group eigenvalue problem with 120 degree symmetry



Pronghorn mesh for PBMR400 Neutronics calculation.

FHR ELS Approach (cont'd)

- *SAM* (System Analysis Module) is being developed at Argonne. The simulation goal of the *SAM* is to provide fast-running, improved-fidelity, whole-plant transient analyses capabilities for SFRs. *SAM* utilizes the object-oriented application framework *MOOSE* and its underlying meshing and finite-element library libMesh, as well as linear and non-linear solvers with PETSc, to leverage modern advanced software environments and numerical methods.
- *SAM* is state of the art for reactor concepts employing single-phase liquid coolants, SFR, MSR, FHR, etc.
- For FHR ELS calculations, *SAM* will provide balance of plant capability.



Flexible multi-scale multi-physics integration through coupling with other M&S tools

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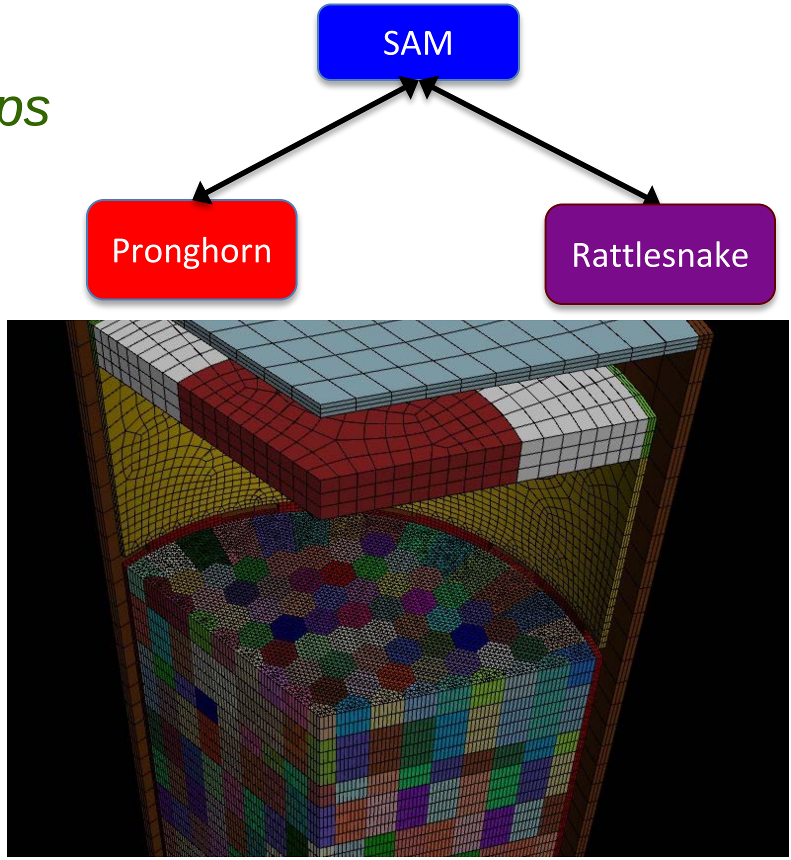
FHR ELS Approach (cont'd)

There are several possible FHR ELS coupling approaches with MOOSE MultiApps and Transfers.

- Choose ***SAM*** as the FHR ELS MasterApp..
- ***Pronghorn*** and ***Rattlesnake*** will serve as MultiApps.
- ***Pronghorn*** will provide homogenized CHT,
- ***Rattlesnake*** will provide power from multi-group diffusion calculations,
- ***and SAM*** will provide balance of plant capability.

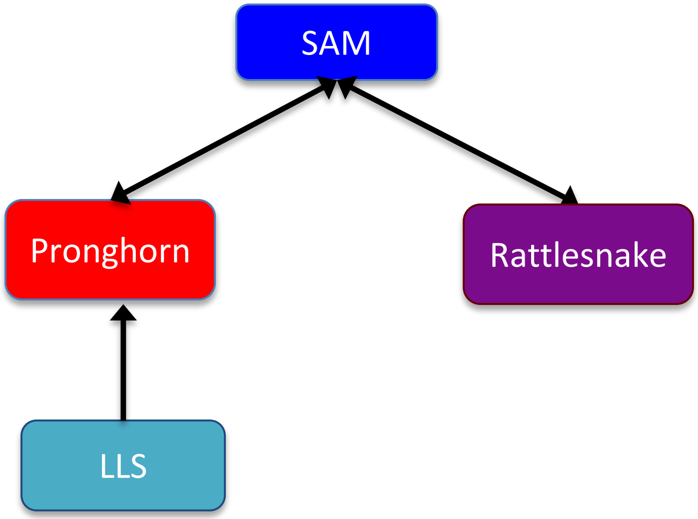


3D Pronghorn Mesh for Prismatic VHTR Concept

FHR ELS Approach (cont'd)

There are several possible FHR ELS coupling approaches with MOOSE MultiApps and Transfers.

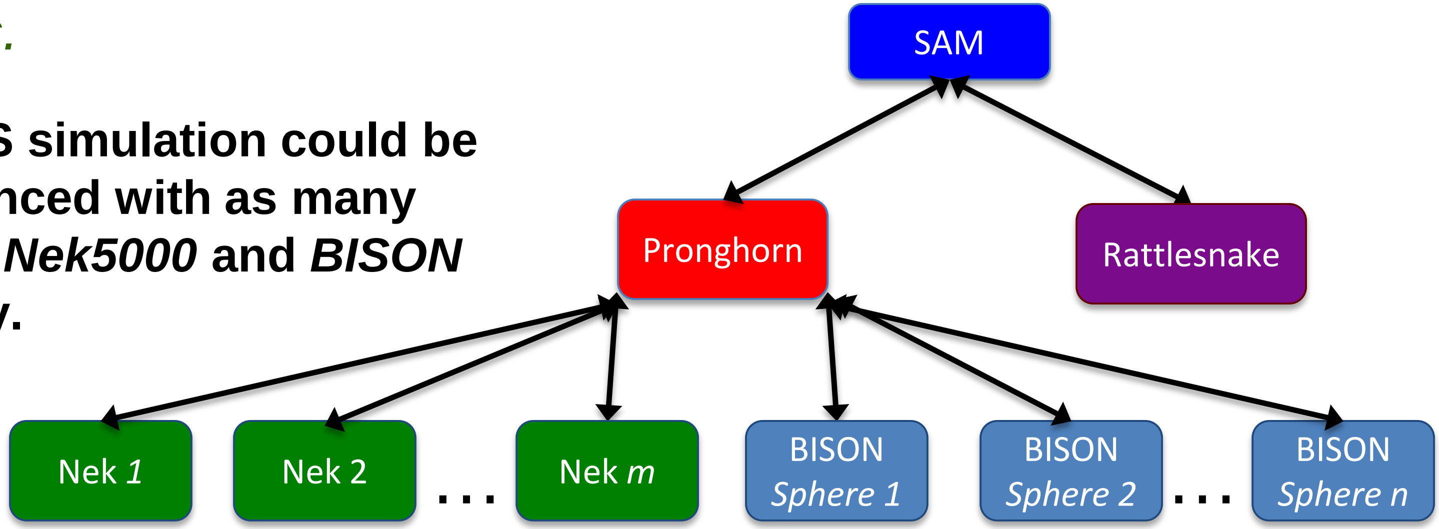
- **Choose *SAM* as the FHR ELS MasterApp..**
- ***Pronghorn* and *Rattlesnake* will serve as MultiApps.**
- ***Pronghorn* will provide homogenized CHT,**
- ***Rattlesnake* will provide power from multi-group diffusion calculations,**
- ***and SAM* will provide balance of plant capability.**
- **The LLS can provide all the closure relations necessary for *Pronghorn* TH model as a one-way transfer.**



FHR ELS Approach (cont'd)

There are several possible FHR ELS coupling approaches with MOOSE MultiApps and Transfers.

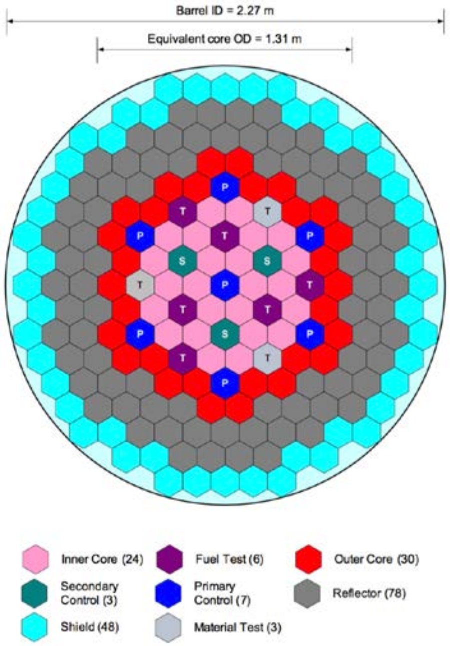
- **The FHR ELS simulation could be further enhanced with as many instances of *Nek5000* and *BISON* as necessary.**

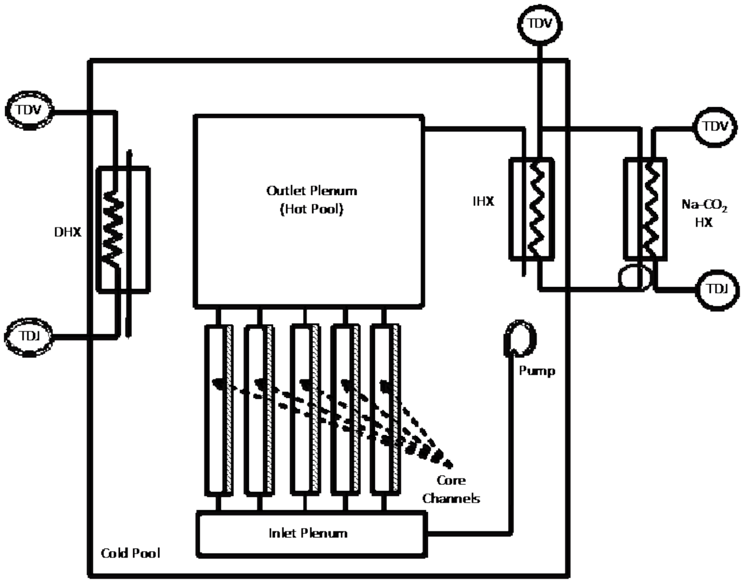


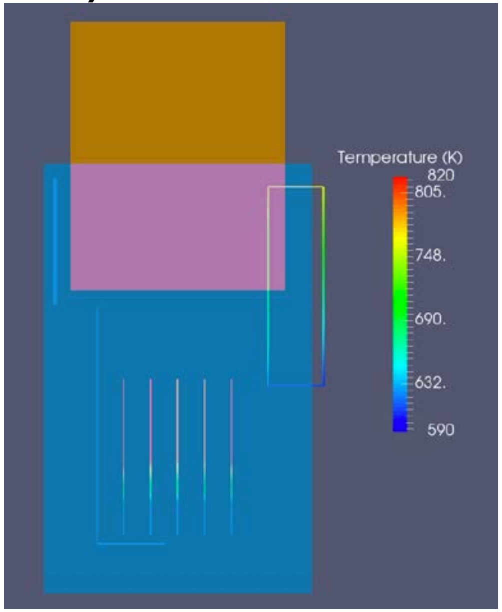
Plant Length Scale Approach

Plant Scale System Thermal-Hydraulics Modeling with *SAM*

- **Robust and high-order FEM model of single-phase fluid flow and heat transfer has been developed and verified;**
  - Component-based code development and system modeling;
- **Flexible coupling capability between fluid and solid components enables a wide range of engineering applications;**
- **Closure Model Enhancements.**







NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

Questions?

NEAMS/SHARP tool set

Elia Merzari (ANL) – ***<u>Slides unavailable</u>***

SAM tool set

Rui Hu (ANL) – ***Slides unavailable***

TRACE/PARCS tool set

Aaron Wysocki (ORNL)

FHR Modeling with TRACE/PARCS

Aaron Wysocki

3/8/2017

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Outline

1. TRACE/PARCS Overview and Modifications
2. Modifications for Molten Salt Reactors (MSRs)
3. Modeling Applications:
   - Fluoride-Salt–Cooled High-Temperature Reactor (FHR) – Demonstration Reactor (DR)
   - Liquid Salt Test Loop (LSTL) at Oak Ridge National Laboratory (ORNL)
   - Advanced High-Temperature Reactor (AHTR)

Implementation of Salts in TRACE

- The TRAC-RELAP Advanced Computational Engine (TRACE) is a best-estimate reactor systems analysis code developed by the US Nuclear Regulatory Commission (NRC), for analyzing transient and steady-state neutronic-thermal-hydraulic behavior in light water reactors (LWRs)
- TRACE can model several different working fluids (H_2O, D_2O, Na, PbBi), as well as multiple noncondensable gas species or predefined mixtures of these gases (air, argon, helium, hydrogen, krypton, nitrogen, xenon, and non-ideal helium)
- Adding liquid salt thermophysical properties to TRACE will enable modeling of the safety performance of Small Modular Advanced High-Temperature Reactors (SmAHTR), (AHTRs), and other salt-cooled reactors

PARCS-TRACE Coupling

- Purdue Advanced Reactor Core Simulator (PARCS) is the US NRC 3D neutronic code
- PARCS couples with TRACE to calculate fuel/moderator/coolant temperatures in steady state and transient conditions
  - 1D axial fluid mass/energy solution
  - 1D radial discretized fuel temperature calculation (cylindrical geometry)
- TRACE is capable of modeling the entire primary and secondary loops:
  - Pumps
  - Heat exchangers
  - Others
- This provides thermohydraulic (TH) feedback to the PARCS neutronic solver
- This coupled neutronic/TH solution gives the best estimate power and temperature distributions

Liquid Salts Selected for Implementation

- Two salts are considered for use as primary coolants:
  - 67% LiF – 33% BeF_2 (FLiBe)
  - 59.5% NaF – 40.5% ZrF_4
- Two salts are considered for use as intermediate loop coolants:
  - 46.5% LiF – 11.5% NaF – 40.5% KF (FLiNaK)
  - 58% KF – 42% ZrF_4

Liquid Salt Thermophysical Properties

- Four thermophysical liquid salt quantities were implemented internally into TRACE
  - Density (temperature-dependent)
  - Viscosity (temperature-dependent)
  - Thermal conductivity (temperature-dependent)
  - Heat capacity (constant)
- These fluid properties were incorporated via function calls in which temperature-dependent constitutive relations are entered directly, and no external tables are used
- Vapor properties, saturation line, surface tension, and heats of vaporization are ***not*** implemented
  - ONLY single-phase conditions without phase changes allowed
  - Must disable phase changes in TRACE calculation, understand liquid operating range of salts

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Melting and Boiling Temperatures

Salt Constituents	Molar Composition (%)	T_{melt} (° C)	T_{boil} (° C)	Source
LiF-BeF_2	67–33	458	~1,400	(5)
KF-ZrF_4	58–42	390	~1,450	(6)
NaF-ZrF_4	59.5–40.5	500	~1,350	(5)
LiF-NaF-KF	46.5–11.5–42	454	1,570	(5)

J. Richard et al., “Implementation of Liquid Salt Working Fluids Into TRACE,” *ICAPP 2014*, Paper 14214, Charlotte, USA, 2014.

Liquid Salt Properties: Density

Salt Constituents	Density Equation	Units	Uncertainty (%)
LiF-BeF_2	$\rho = -0.4884 \cdot T + 2413$	T in K, ρ in kg/m^3	±0.05
KF-ZrF_4	$\rho = -0.887 \cdot T + 3658$	T in K, ρ in kg/m^3	±5
NaF-ZrF_4	$\rho = -0.889 \cdot T + 3827$	T in K, ρ in kg/m^3	±2
LiF-NaF-KF	$\rho = -0.73 \cdot T + 2729$	T in K, ρ in kg/m^3	±2

- Density is the most well-characterized fluid property
- Linear dependence on temperature is observed throughout liquid operating range
- No pressure-dependent terms were reported, but they are required by TRACE and are approximated as 1E-7 $kg/m^3/Pa$

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Liquid Salt Properties: Viscosity

Salt Constituents	Viscosity Equation	Units	Uncertainty (%)
LiF-BeF_2	$\mu = 1.16 \cdot 10^{-4} \cdot e^{3775/T}$	T in K, μ in Pa-s	±20
KF-ZrF_4	$\mu = 1.59 \cdot 10^{-4} \cdot e^{3179/T}$	T in K, μ in Pa-s	±20
NaF-ZrF_4	$\mu = 7.67 \cdot 10^{-5} \cdot e^{3977/T}$	T in K, μ in Pa-s	±20
LiF-NaF-KF	$\mu = 4.0 \cdot 10^{-5} \cdot e^{4170/T}$	T in K, μ in Pa-s	±20

- Viscosity varies more with temperature than any other fluid property
- Salts are Newtonian fluids exhibiting exponential decrease in viscosity with reciprocal temperature
- Measurement uncertainty is poor; newer measurements would be valuable

Liquid Salt Properties: Thermal Conductivity

Salt Constituents	Formula Weight (g/mol)	Thermal Conductivity Equation	Units	Uncertainty (%)
$LiF\text{-}BeF_2$	33.0	$k = 0.0005 \cdot T + 0.63$	T in K, k in W/m-K	±15
$KF\text{-}ZrF_4$	103.9	$k = 0.0005 \cdot T + 0.032$	T in K, k in W/m-K	±15
$NaF\text{-}ZrF_4$	92.7	$k = 0.0005 \cdot T + 0.0052$	T in K, k in W/m-K	±15
LiF-NaF-KF	41.3	$k = 0.0005 \cdot T + 0.43$	T in K, k in W/m-K	±15

- Difficult to measure; results are in large uncertainties
- Ignatiev’s empirical correlation is used to estimate thermal conductivity

Liquid Salt Properties: Heat Capacity

Salt Constituents	Molar Composition (%)	Heat Capacity (J/kg-K)	Uncertainty (%)
$LiF\text{-}BeF_2$	67–33	2416	±2
$KF\text{-}ZrF_4$	58–42	1051	±20
$NaF\text{-}ZrF_4$	59.5–40.5	1172	±10
LiF-NaF-KF	46.5–11.5–42	2010	±20

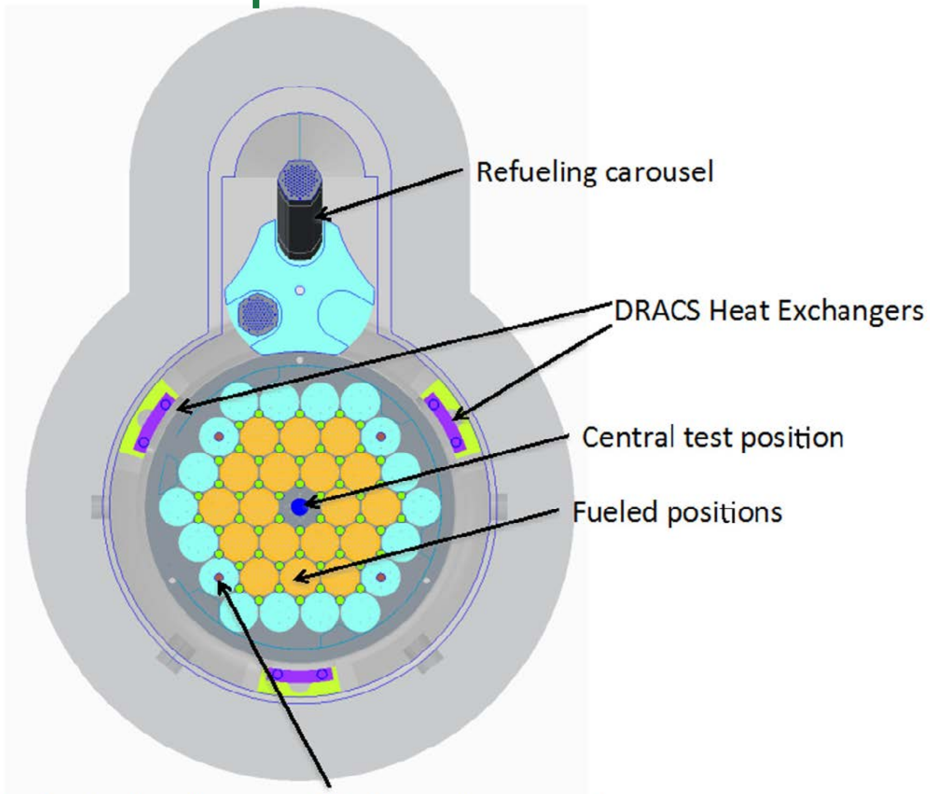
- Temperature dependence is small, indistinguishable from measurement error
- Constant heat capacity values are used in TRACE
- All values obtained from experiments except $KF\text{-}ZrF_4$, which was estimated using the empirical Dulong-Petit approach

Modeling Applications: FHR-DR

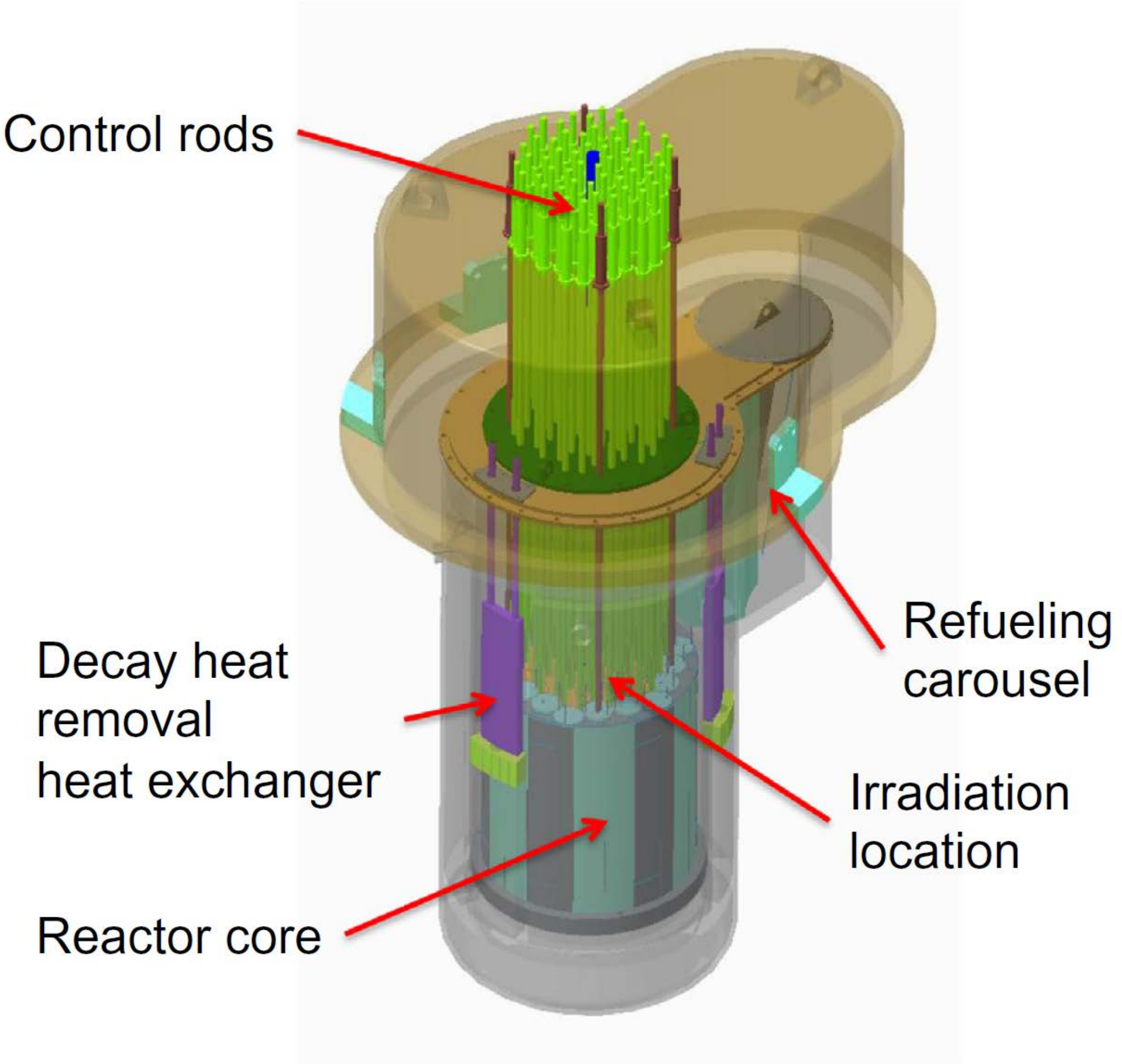
FHR Demonstration Reactor

- Preconceptual design; 100 MWth
- TRISO fuel embedded in prismatic graphite blocks
- Tube-and-shell primary-to-intermediate heat exchangers; passive DRACS

Top View



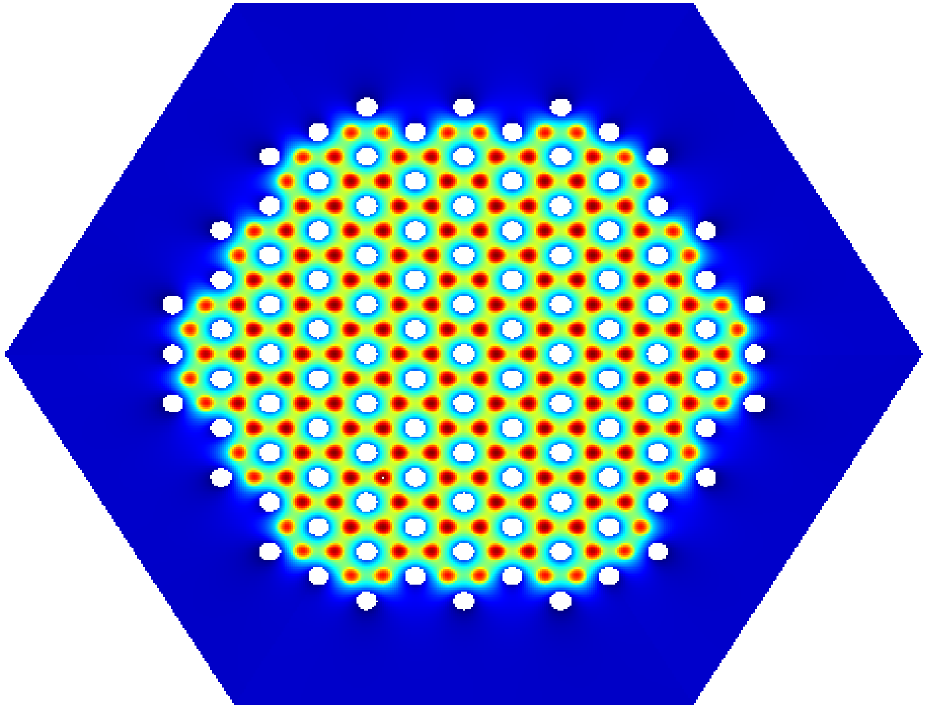
Side View



L. Qualls et al., "Preconceptual design of a fluoride high temperature salt-cooled engineering demonstration reactor: Motivation and overview," *Ann. Nucl. Energy,* vol. 103, 49-–59, 2017.

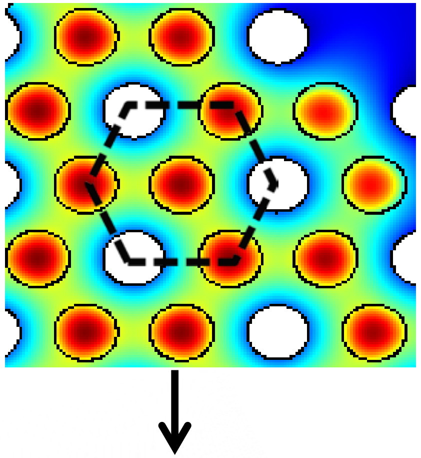
FHR-DR Prismatic Temperature Calculation

Detailed Temperature Calculation (from COMSOL)



Simplified Temperature Calculation in Systems Codes (PARCS, TRACE, RELAP)

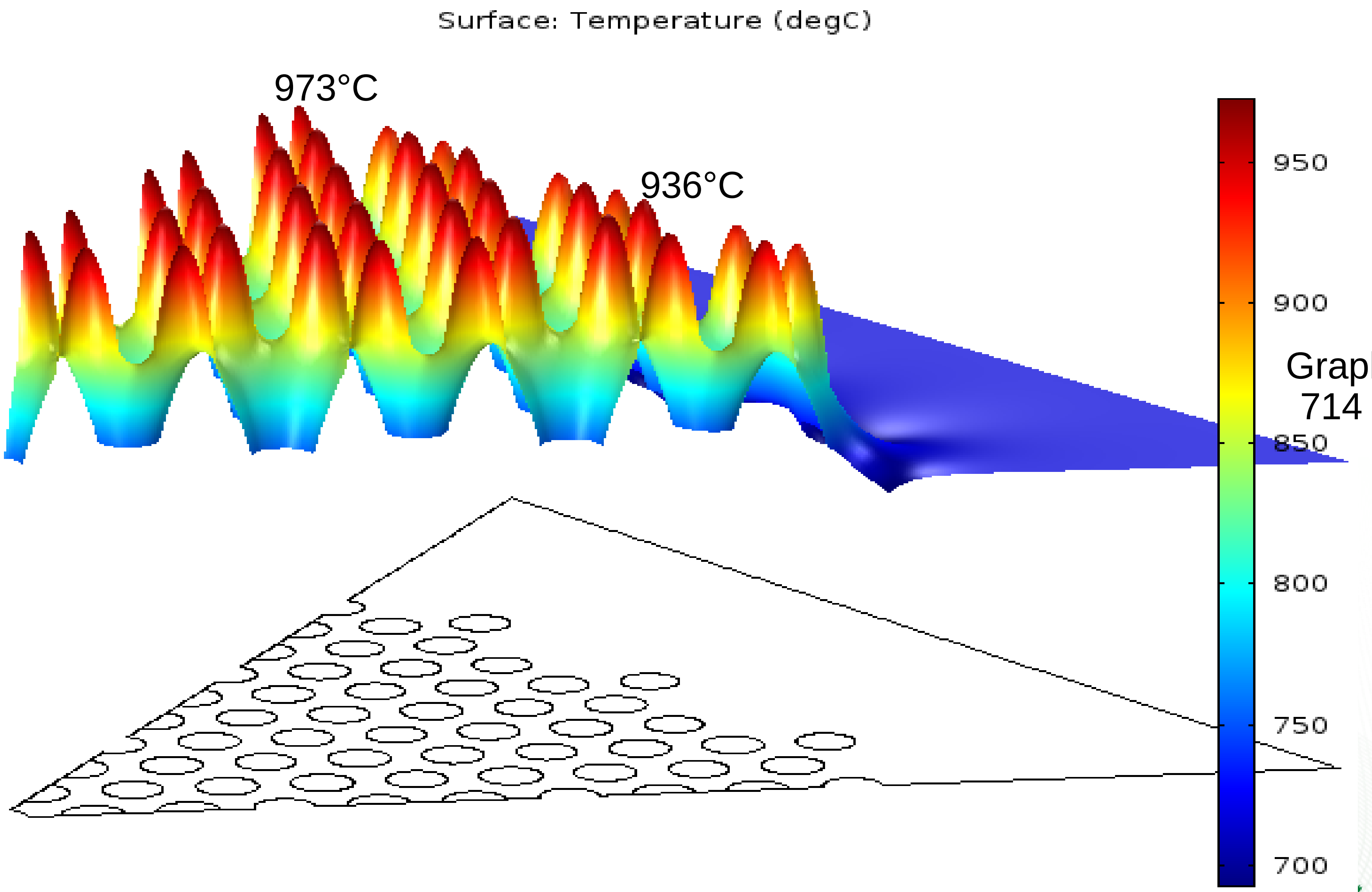
- Reduce the detailed geometry to an equivalent subassembly, preserving the total flow area and fuel volume
- Graphite thickness can be adjusted to give the right fuel temperatures



Red: fuel
Green: graphite
Gray: coolant

N. Brown et al., "Preconceptual design of a fluoride high temperature salt-cooled engineering demonstration reactor: Core design and safety analysis," *Ann. Nucl. Energy,* vol. 103, 49-–59, 2017.

COMSOL Detailed Temperature Calculation



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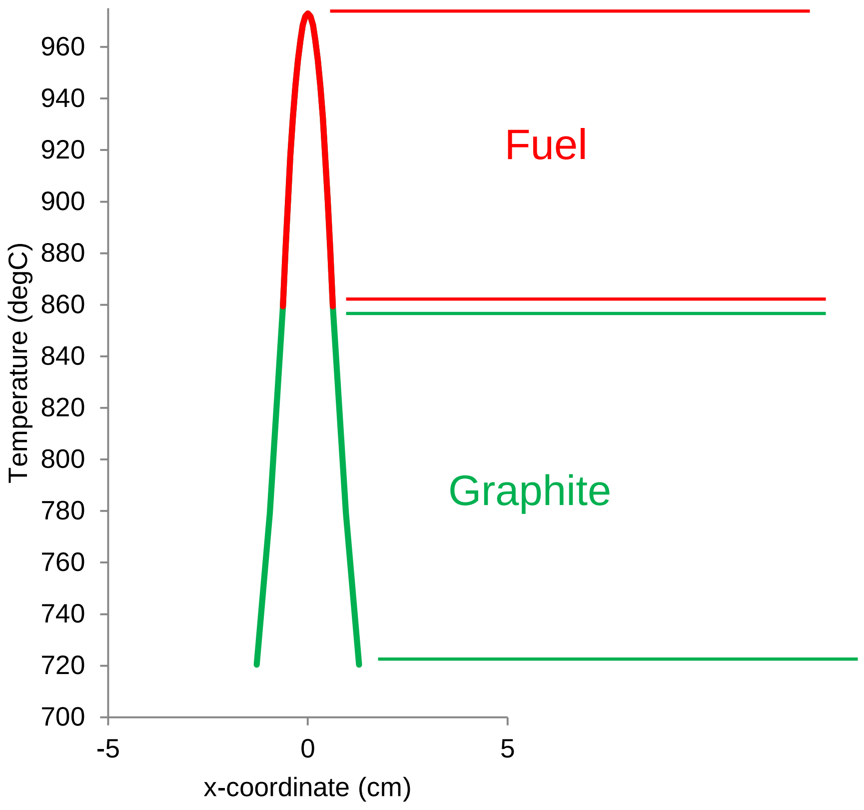
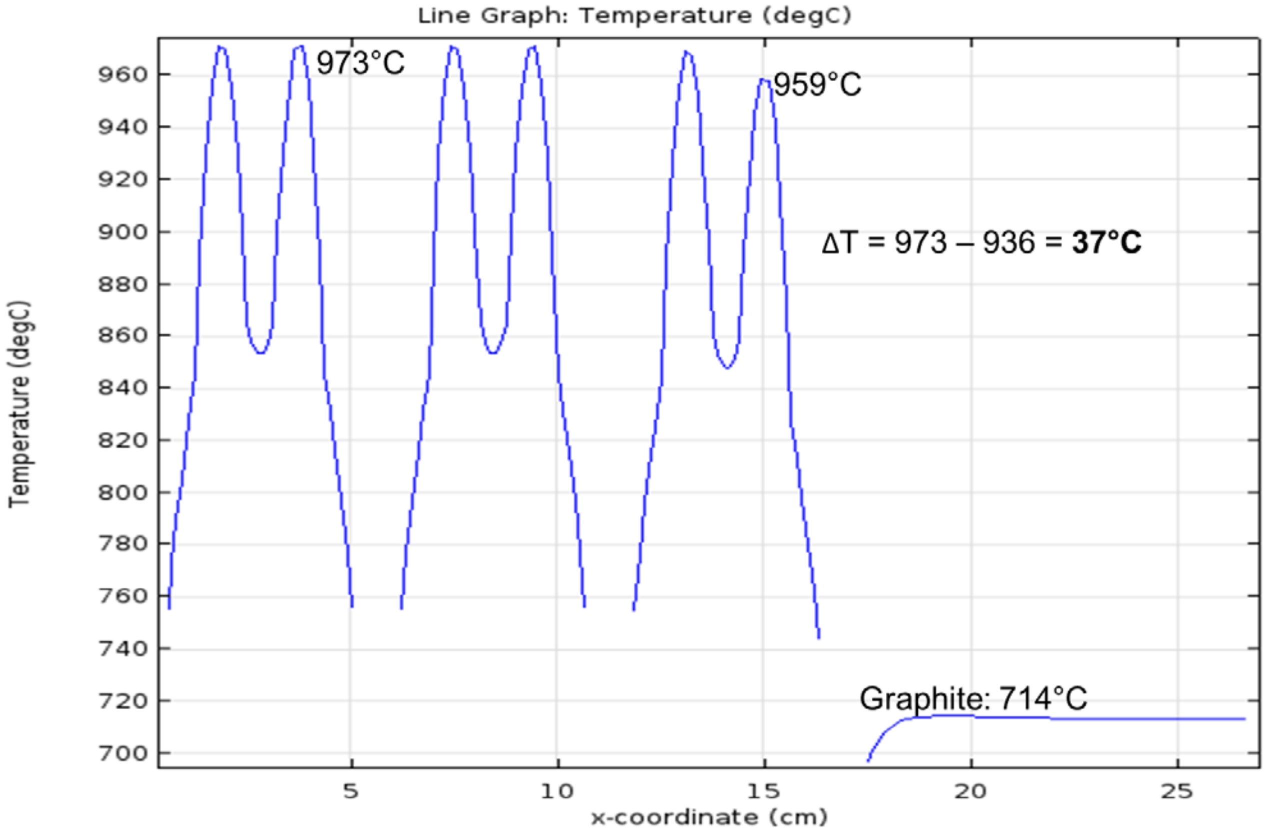
Fuel/Graphite Temperature Comparison

The PARCS graphite thickness has been adjusted to match the average fuel and graphite temperatures in COMSOL

PARCS Results

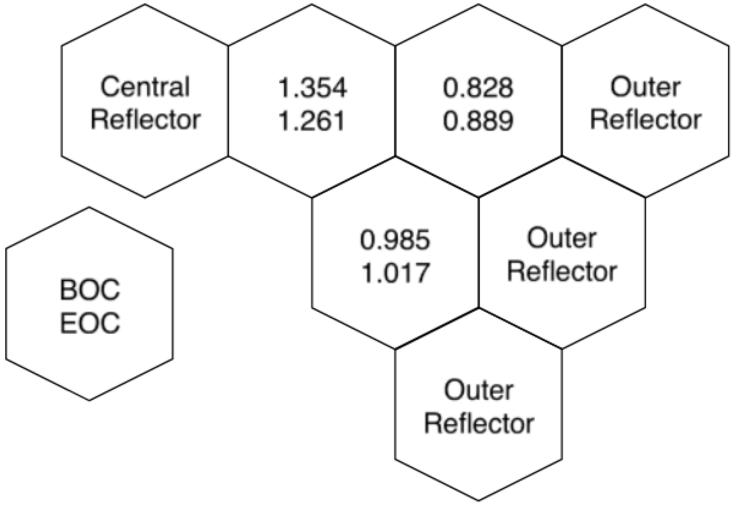


COMSOL Results

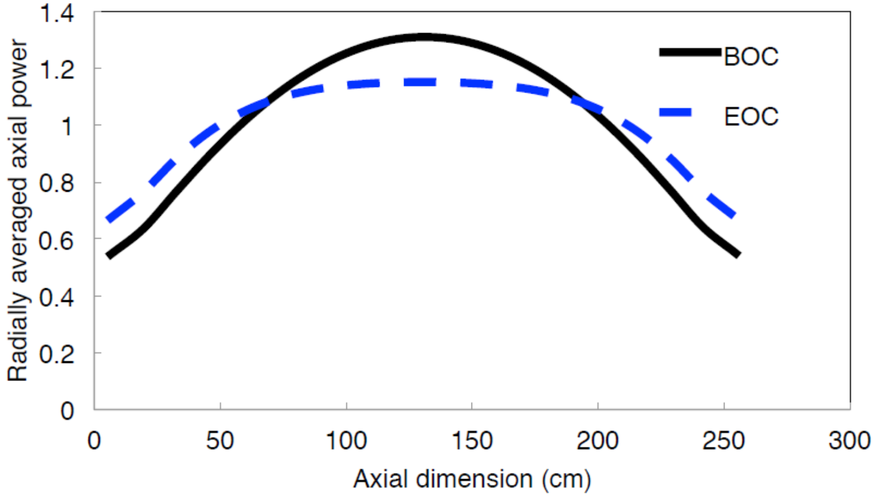


PARCS FHR-DR Steady State Results

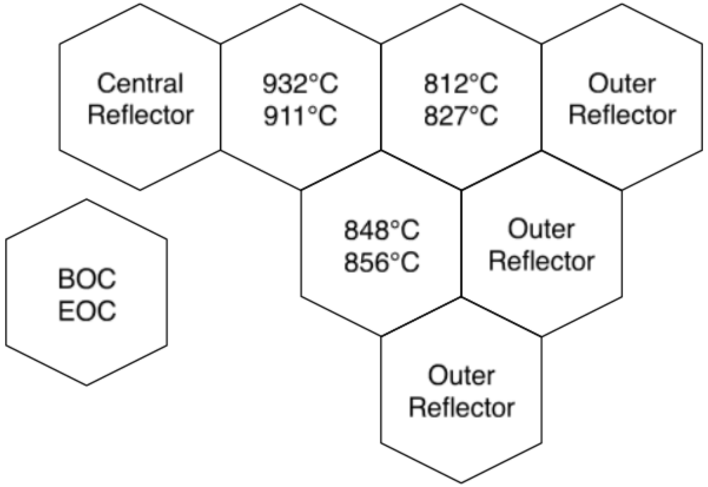
Radial Assembly Power Distribution



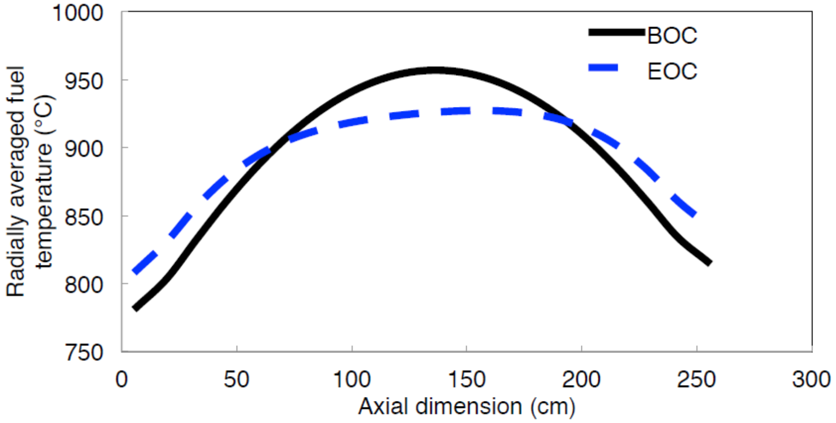
Average Axial Power Distribution



Radial Fuel Temperature Distribution

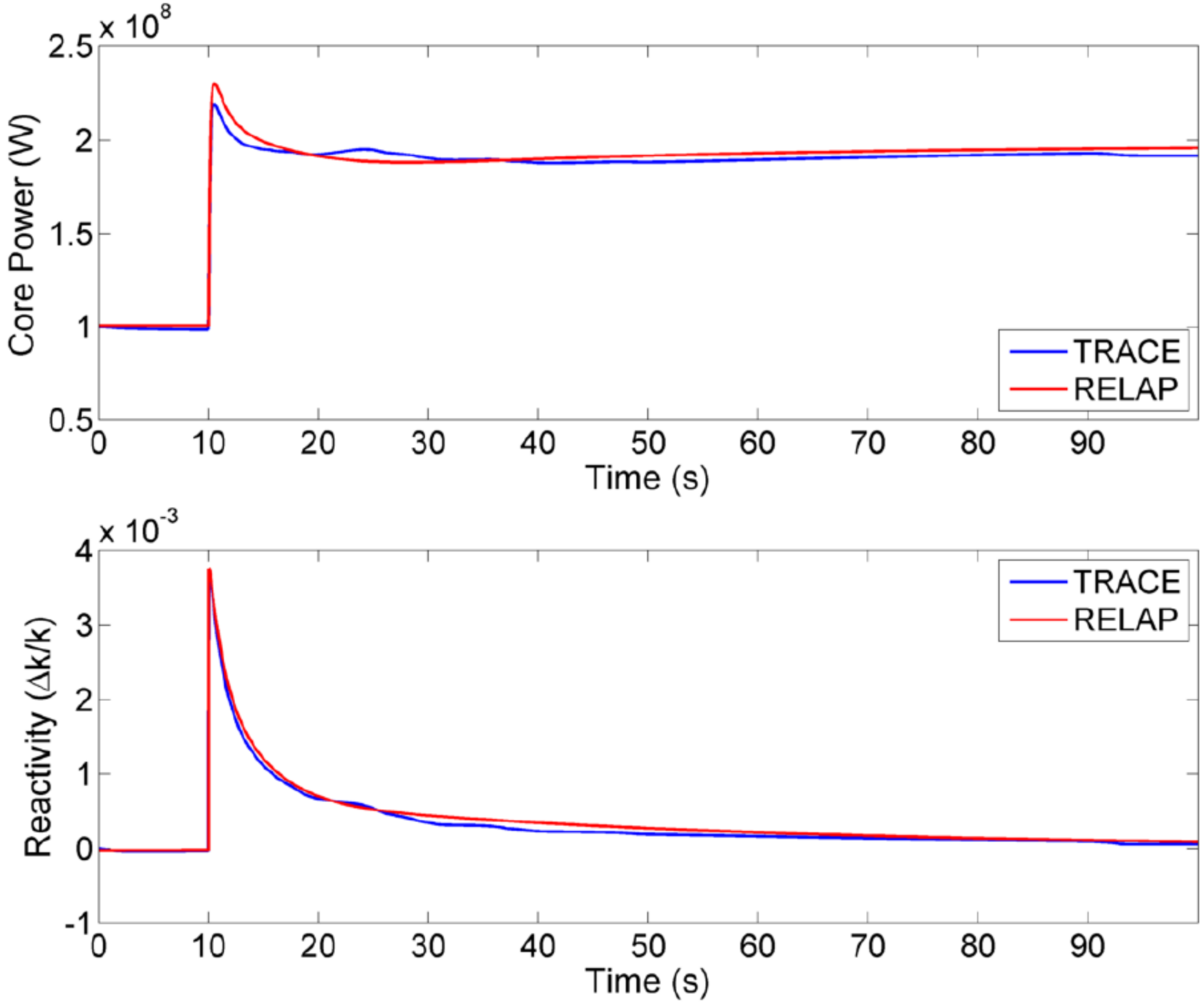


Average Axial Fuel Temperature Distribution

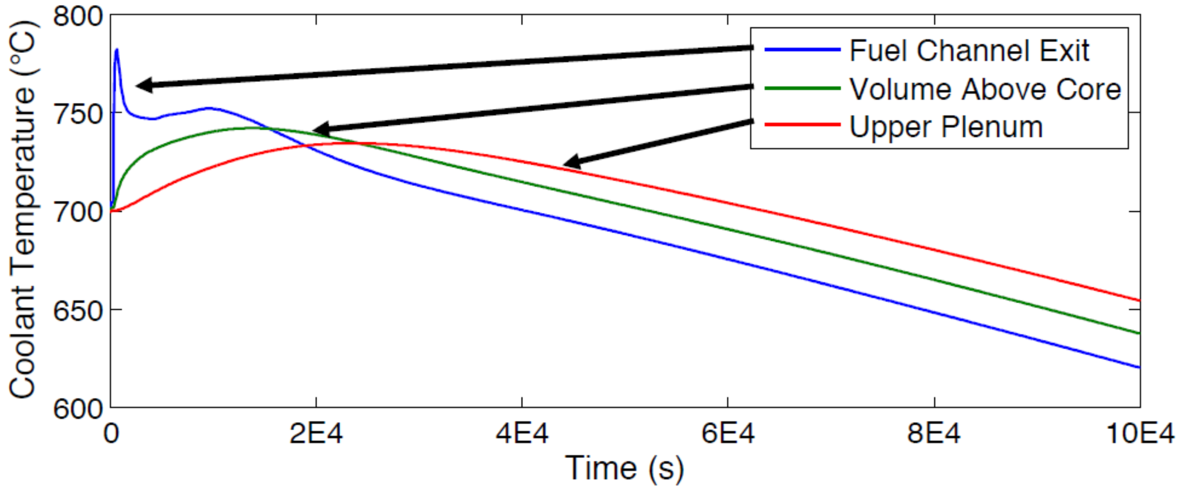


FHR-DR Transient Simulations

Hot Full Power (HFP) Rapid Rod Withdrawal

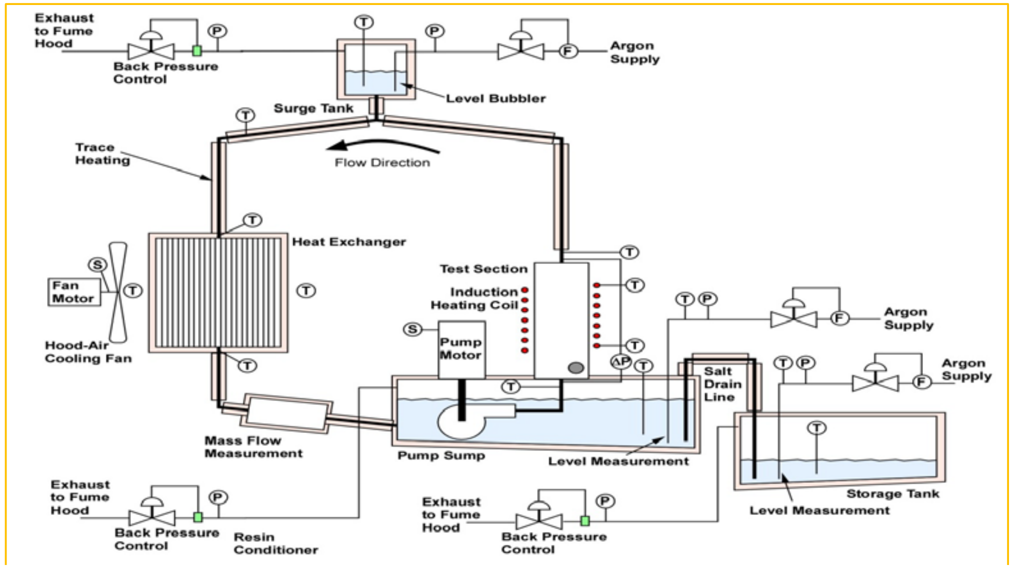


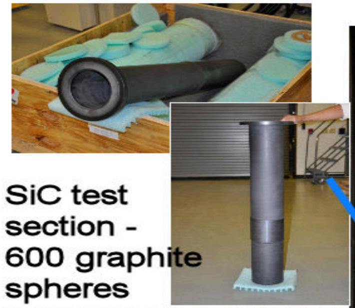
Loss of Forced Flow (LOFF) with Scram



Modeling Applications: ORNL LSTL

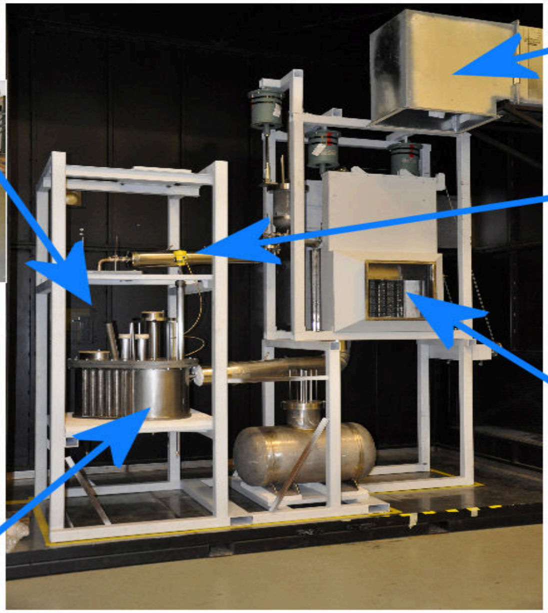
A TRACE Model of the ORNL LSTL Has Been Developed





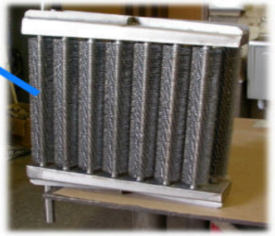
SiC test section - 600 graphite spheres 1.25 kw/sphere (max)

Overhung shaft Centrifugal sump pump

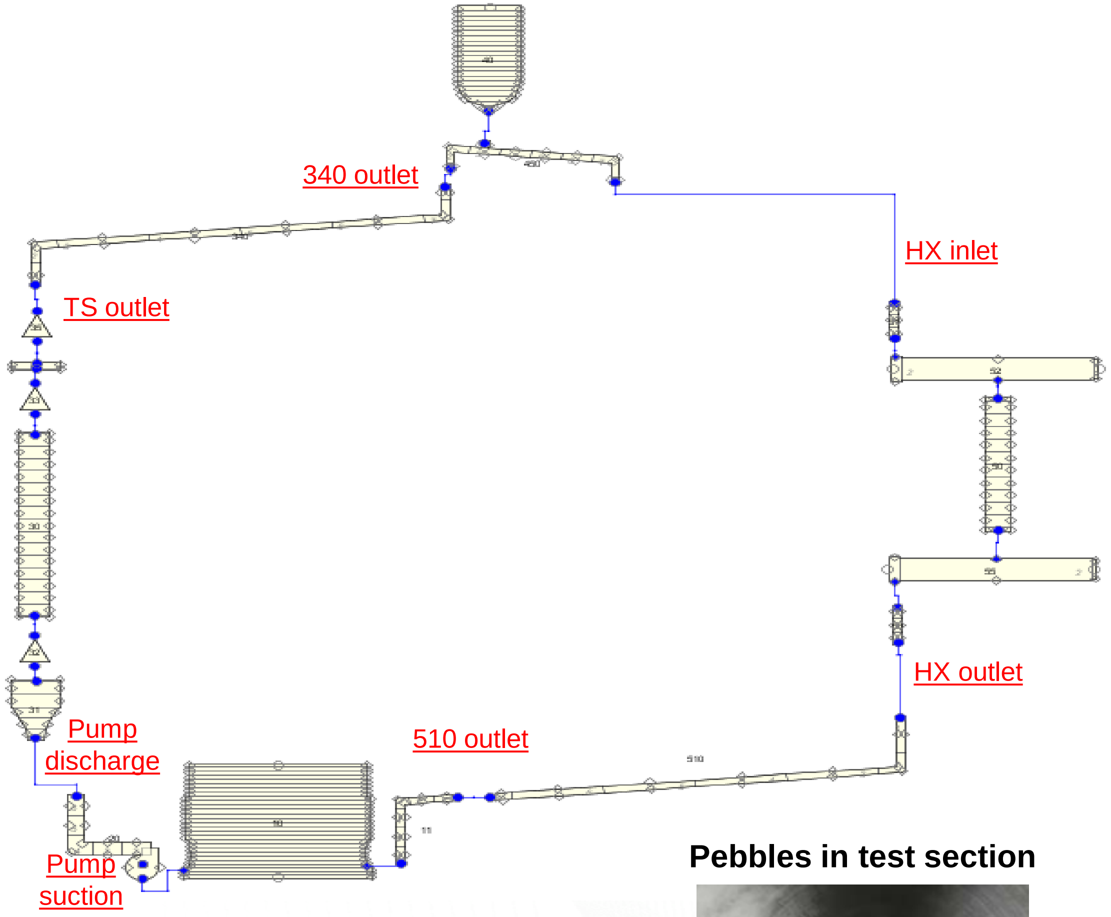


Variable Speed Air Supply

Radar based level detector



Finned tube air cooler - 200 kw



Pebbles in test section

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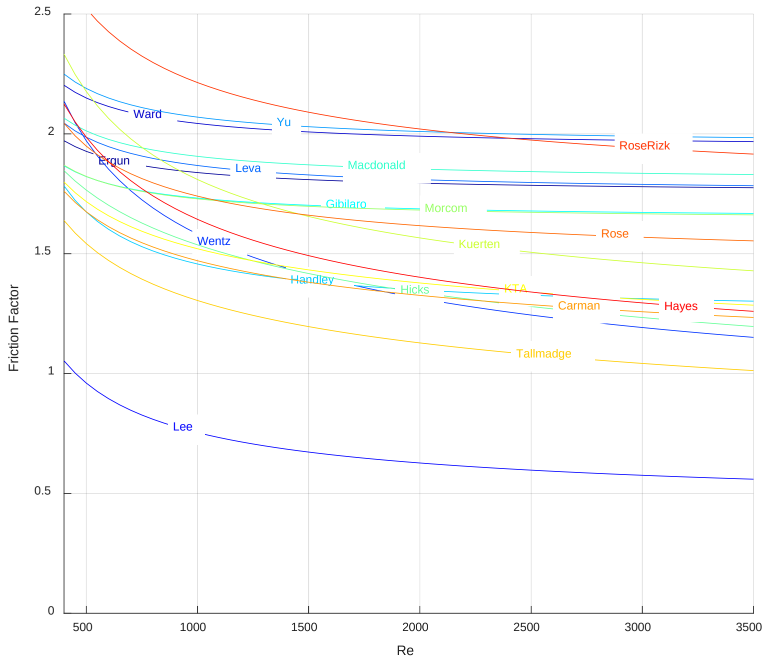
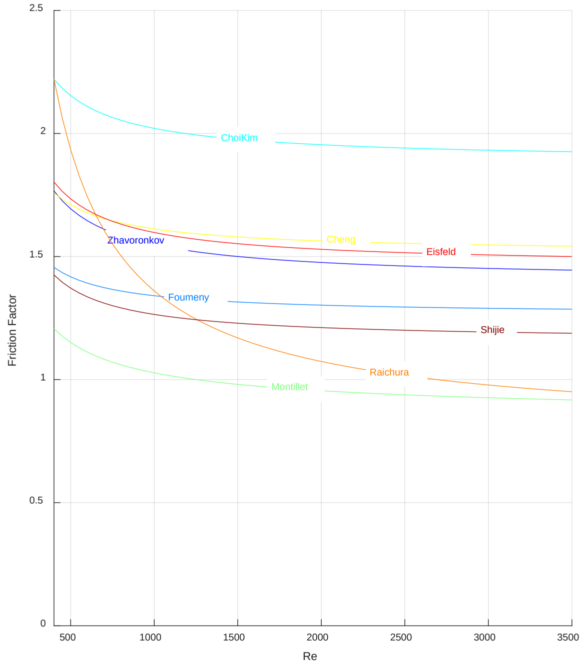
Pebble Bed Friction Correlations





Correlations that do not account for wall

- Each experiment at different ptb diameter ratio

Most used correlation: **Ergun**

- Overprediction of results
- The wall effect is not accounted for, but might not be the only reason

$$f = \frac{150}{Re_p} * (1 - \epsilon) + 1.75$$

Correlations that account for wall:

- Ptb diameter ratio
- Plot assumes Dratio = 5

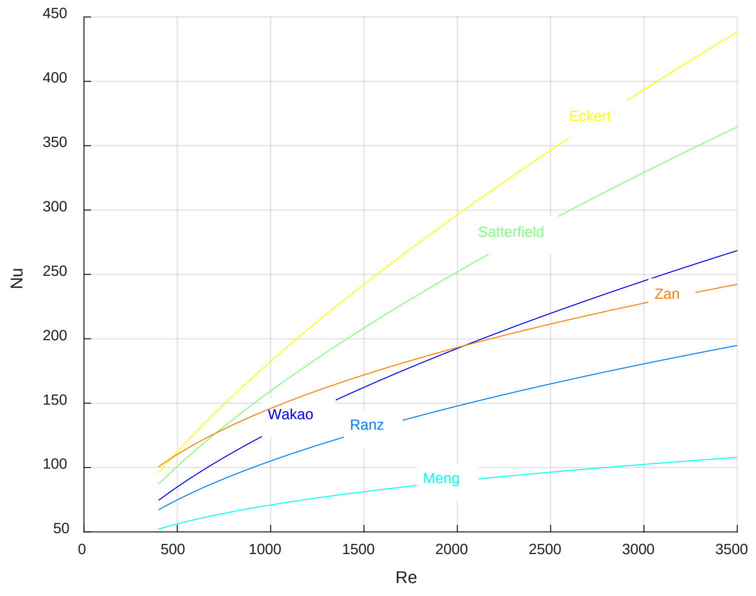
Most promising correlation: **Eisfeld**

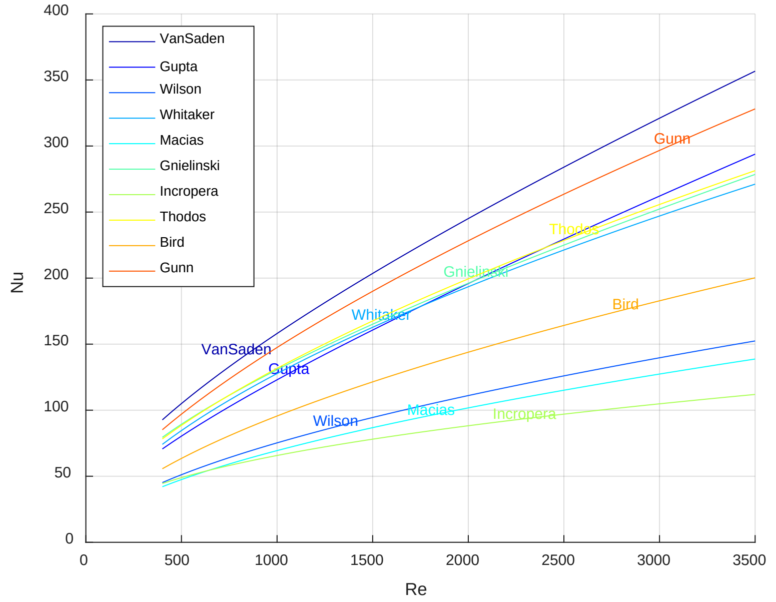
- Combines the wall friction and the wall porosity increase

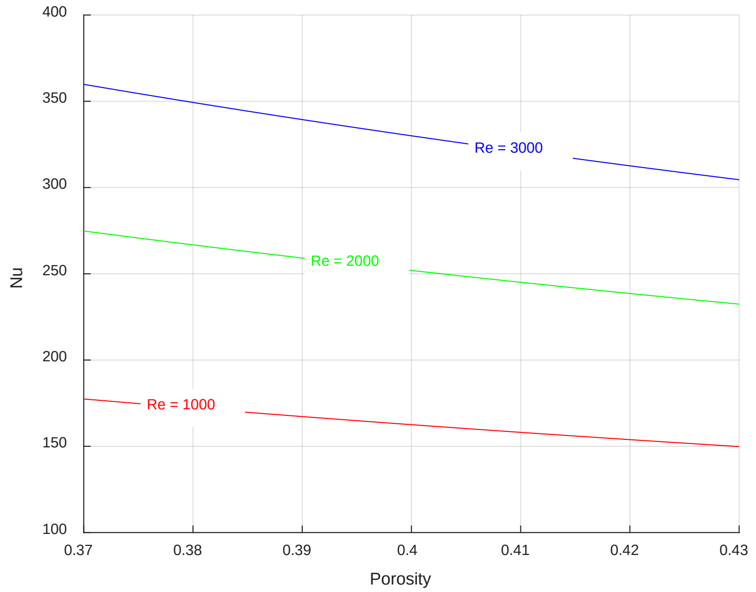
$$f = \frac{154 * M^2}{Re_p} * (1 - \epsilon) + \frac{M}{B_e}$$

P. Avigni, A. Wysocki, and G. Yoder, "Liquid Salt Test Loop Modeling using TRACE," *Ann. Nucl. Energy,* in review, submitted Nov 2016.

Pebble Bed Heat Transfer Correlations







Not accounting for bed porosity

Most common correlation: **Wakao**

Debate on low Re behavior

- Nu should go to 0 for Re -> 0
- Nu is constant and equal to the single sphere Nu in absence of flow

$$Nu = 2 + 1.1 * Pr^{\frac{1}{3}} * Re_p^{0.6}$$

Accounting for bed porosity

Selected correlation: **van Saden** (KTA)

Dependence on porosity:

- 1% variation in porosity results in 3% variation in Nu
- Not dependent on Re

$$Nu_p = 1.27 * \frac{Pr^{0.33} * Re_p^{0.36}}{\epsilon^{1.18}} + 0.033 * \frac{Pr^{0.5} * Re_p^{0.86}}{\epsilon^{1.07}}$$

Implementation of Pebble Bed Correlations in TRACE

The following correlations have been implemented in TRACE:

Friction correlations:

- Ergun correlation
- Eisfeld correlation (ptb diameter ratio dependence)

Heat transfer correlations:

- Wakao correlation
- Van Saden correlation (porosity dependence)

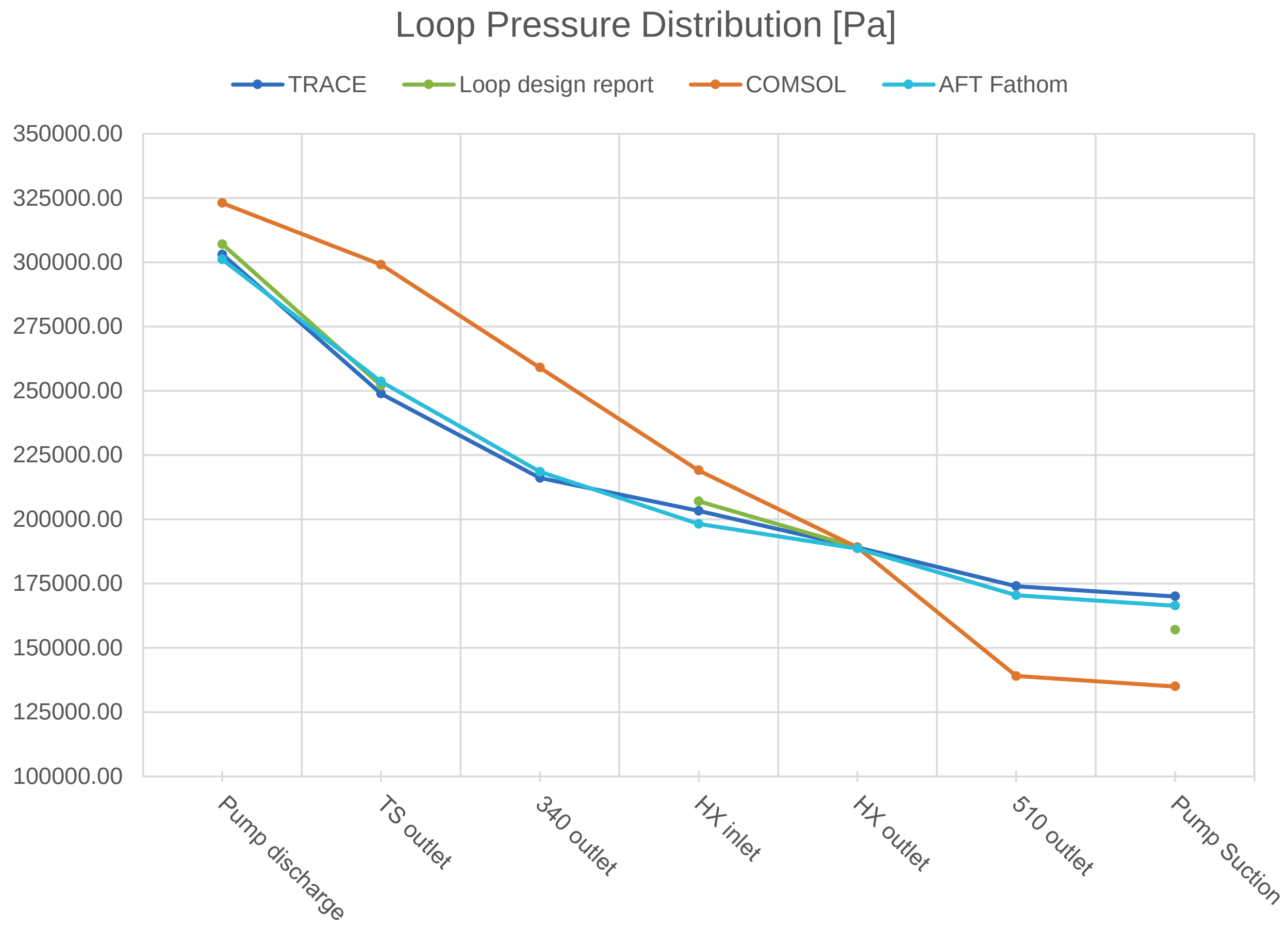
Comments on friction correlations:

- Implemented for the pipe component only
- Not available for 3D components
- User is required to enter array of porosity and pebble diameter for each pipe with pebbles

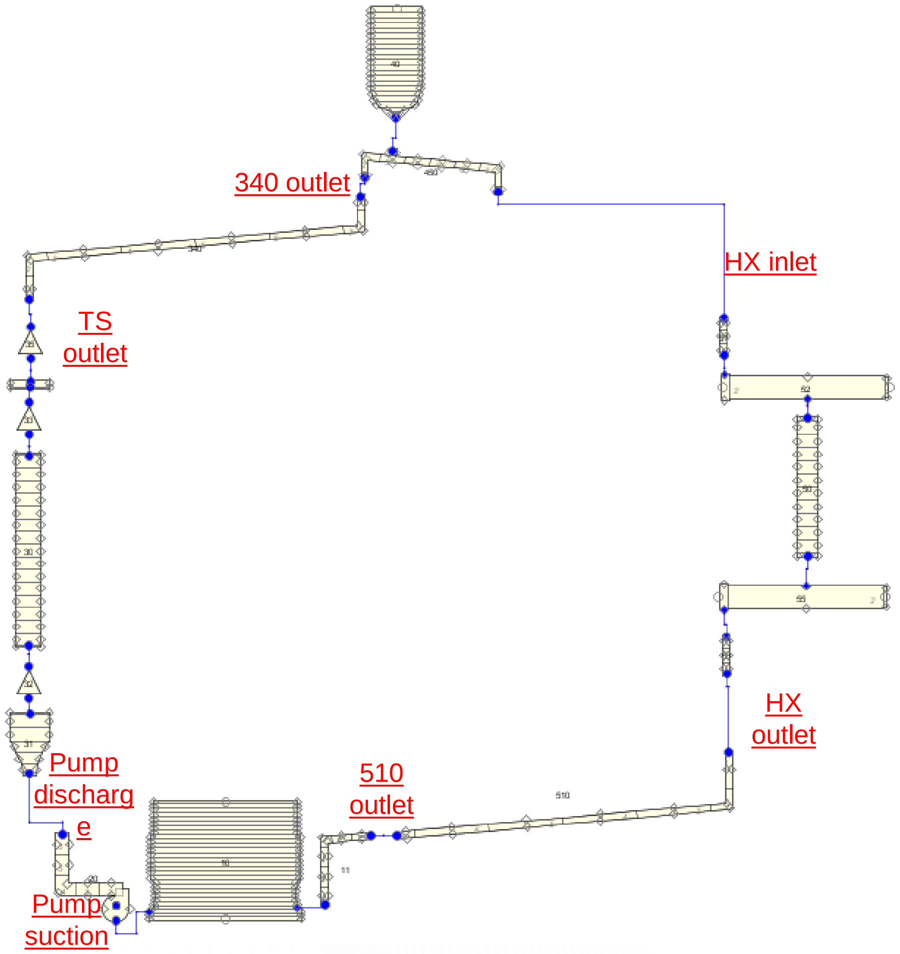
Comments on heat transfer correlations:

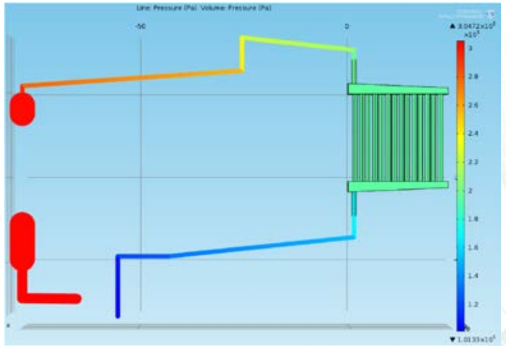
- HT correlations implemented for heat structure component
- User required to enter porosity and pebble diameter for each heat structure with pebbles

Loop Pressure Distribution



Overall TRACE pressure drop is equal to 0.14 Mpa





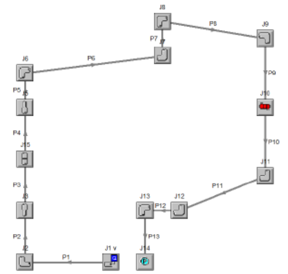


Figure 27. AFT Fathom model of the LSTL.

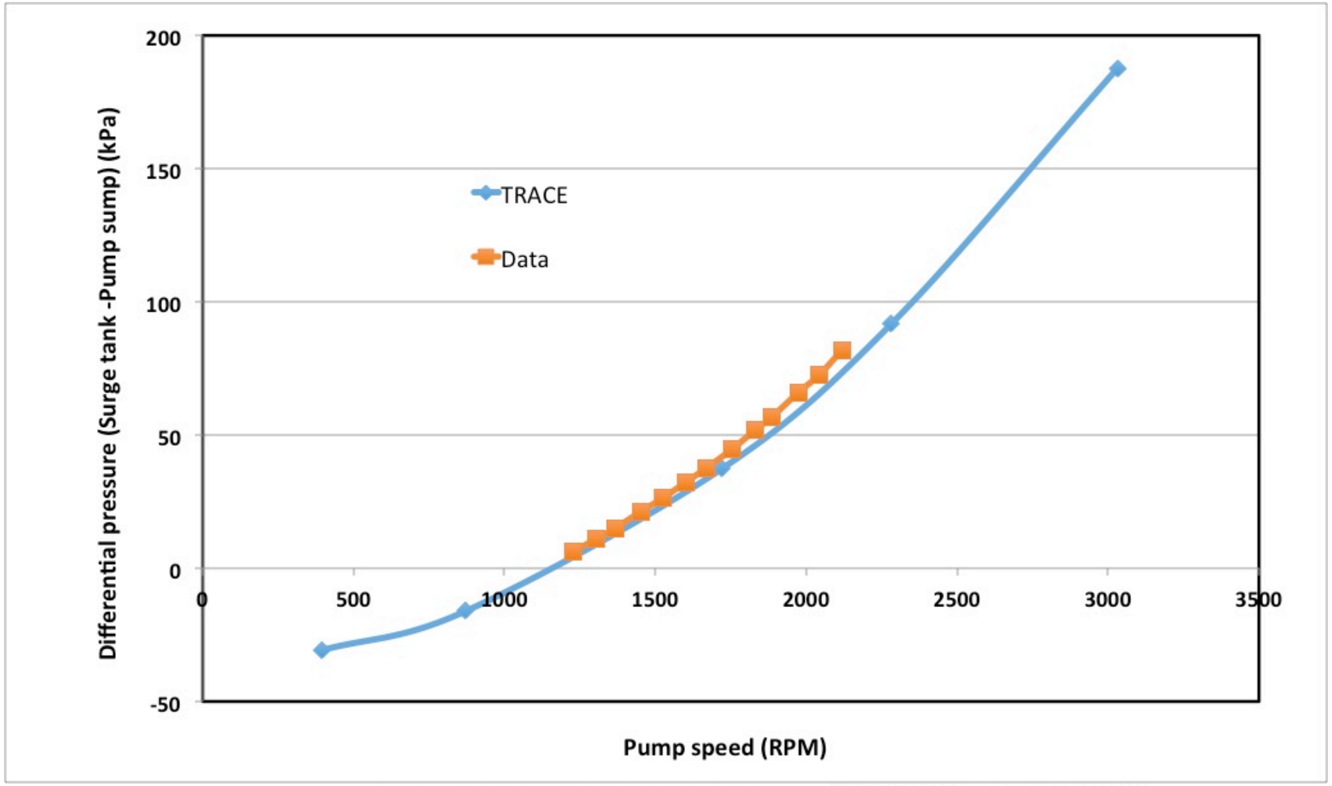
Initial Comparison of TRACE Predictions Have Been Made with LSTL Data

Surge Tank Gas P

Pebble Bed
Test Section

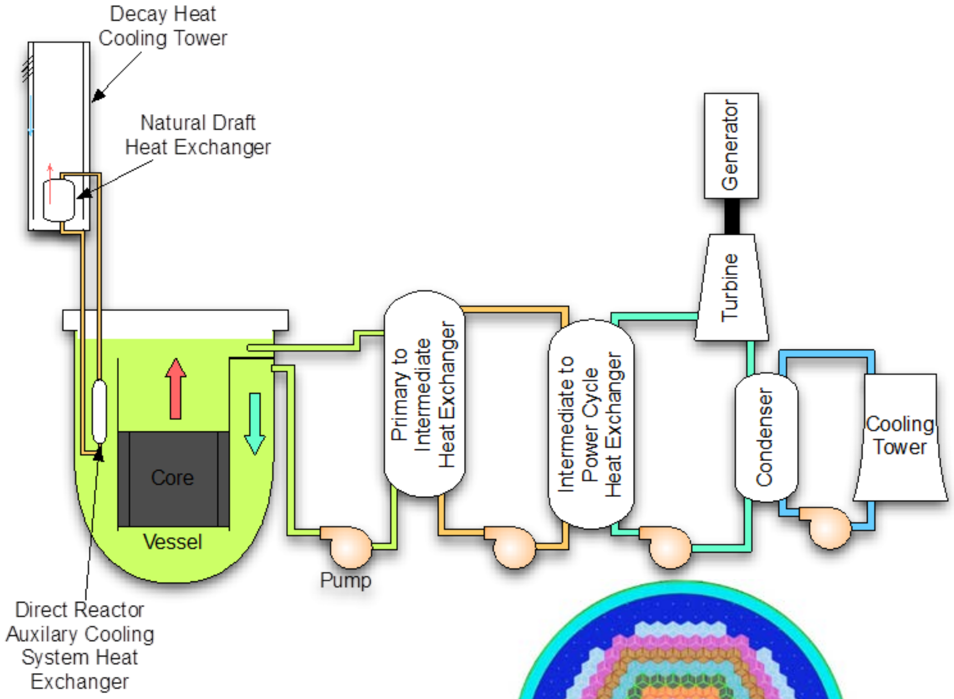
Pump

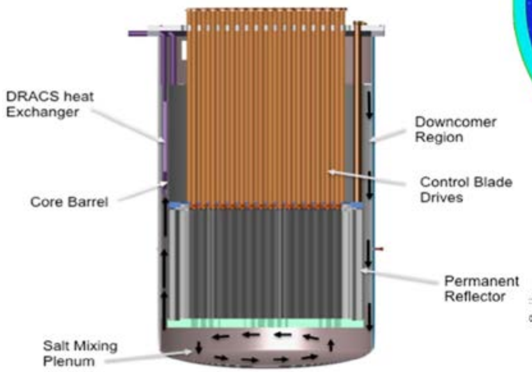
Sump Tank Gas P

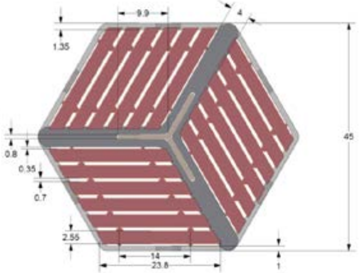


Modeling Applications: AHTR

AHTR Design

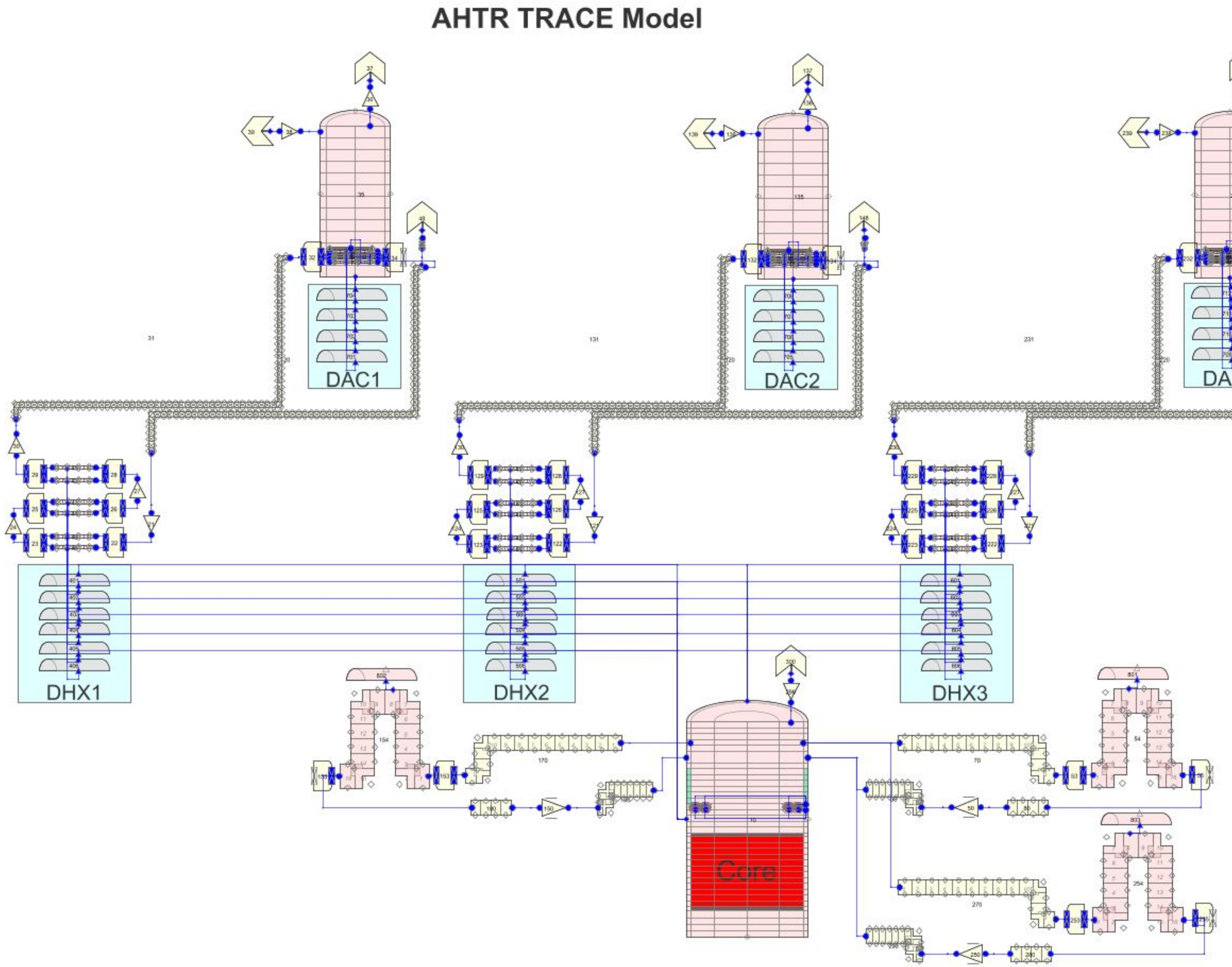






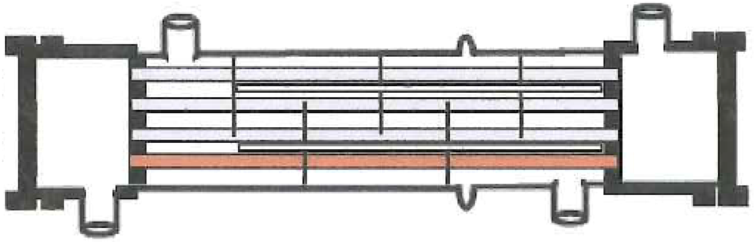
- The Advanced High Temperature Reactor is a molten salt cooled reactor design concept, which is intended to safely, efficiently and economically produce large amounts of electricity with minimal impact on the environment.
- The AHTR features low pressure molten fluoride salt coolant, a carbon-carbon composite fuel form featuring compacts of coated particle fuel, and fully passive decay heat rejection.
- An initial baseline mechanical design has been established based on preliminary core design studies, and system dynamics studies.
- Analysis is performed for preconceptual AHTR design

TRACE ATHR Model



D. Wang et al., “Thermal hydraulics analysis of the Advanced High Temperature Reactor,” *Nuc. Eng. and Des.*, vol. 294, 73–85, 2015.

Primary Heat Exchanger (PHX) Design and Modeling



	Option 1		Option 2		Option3	
	Tube	Shell	Tube	Shell	Tube	Shell
Loop Allocation	Primary	Interm.	Interm.	Primary	Primary	Interm.
Coolant Salt	FLiBe	$KF\text{-}ZrF_4$	$KF\text{-}ZrF_4$	FLiBe	FLiBe	FLiNaK
Tube Length (m)	20.0					
Tube ID (m)	0.019735					
Tube Wall Thickness (m)	0.001245					
# of tubes	20000		18000		12000	
Tube Pitch (m)	1.5 OD					
Tube Arrangement	Square					
Shell Inside Diameter (m)	5.44		5.18		4.26	
Baffle Spacing (m)	2.0					
Baffle Cut	25%					
HTC (W/m^2-K)	2853.3	2530.5	2116.9	5044.3	4768.8	4387.4
Pressure Drop (Pa)	2.10E+04	1.23E+6	3.55E+04	8.92E+5	5.26E+04	6.04E+5
PHX Pumping Power (MW)	0.10	6.24	0.18	4.35	0.26	2.20

Oak Ridge National Laboratory

PHX Heat Transfer (HT) and Pressure Drop Correlations

Heat transfer correlation for staggered tube bundle:

$$Nu = 1.04Re^{0.4}Pr^{0.36}(\frac{Pr}{Pr_w})^{0.25} \qquad 1 \leq Re < 5\times10^2$$

$$Nu = 0.71Re^{0.5}Pr^{0.36}(\frac{Pr}{Pr_w})^{0.25} \qquad 5\times10^2 \leq Re < 10^3$$

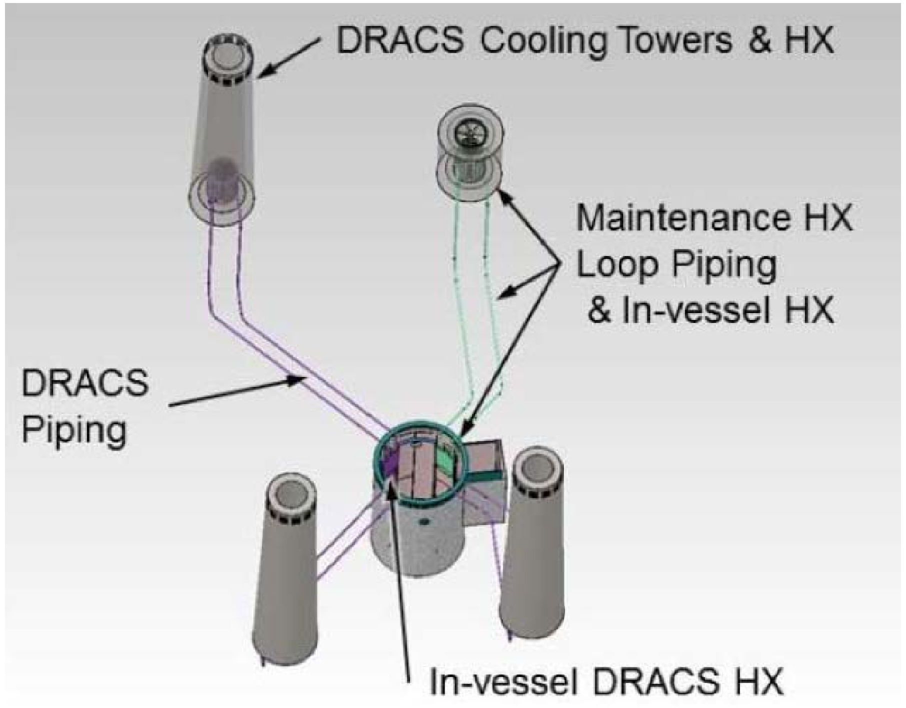
$$Nu = 0.35(X_t^*/X_l^*)^{0.2}Re^{0.6}Pr^{0.36}(\frac{Pr}{Pr_w})^{0.25} \qquad 10^3 \leq Re < 2\times10^5$$

$$Nu = 0.031(X_t^*/X_l^*)^{0.2}Re^{0.8}Pr^{0.36}(\frac{Pr}{Pr_w})^{0.25} \qquad 2\times10^5 \leq Re < 2\times10^6$$

Pressure drop correlation for staggered configuration:

$$\Delta P = \xi N_r(\rho V_n^2/2)$$

Direct Reactor Auxiliary Cooling System (DRACS) Design and Modeling – DRACS Heat Exchanger (DHX)

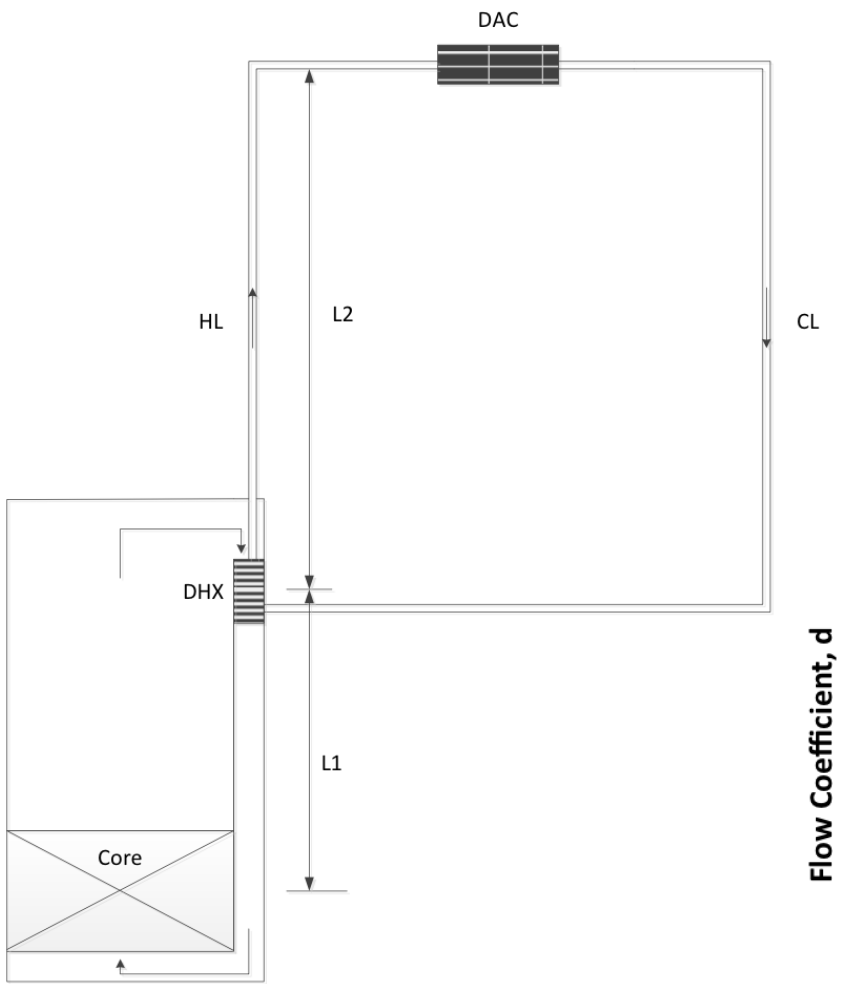


DHX design:	Shell and tube
Tube arrangement:	Staggered
Primary side:	Shell
DRACS side:	tube
# of tubes:	1078
# of tube rows:	98
# of tube passes:	3
Tube length (m):	3.6
Tube OD (m):	0.0254
Tube wall thickness (m):	1.651E-3
Tube material:	Hastelloy N

DRACS Design and Modeling - DAC

DAC design:	Horizontal finned tubes
Tube arrangement	Inline
DRACS loop side:	tube
# of tubes:	200
# of tube rows:	4
# of tube passes:	1
Tube length (m):	4.0
Tube OD (m):	0.0254
Tube wall thickness (m):	1.651E-3
Fin height (m):	0.0254
Fin spacing (m):	0.015
Transverse tube spacing (m):	0.0802
Longitudinal tube spacing (m):	0.0802
Tube material:	Hastelloy N

DRACS Design and Modeling - DAC

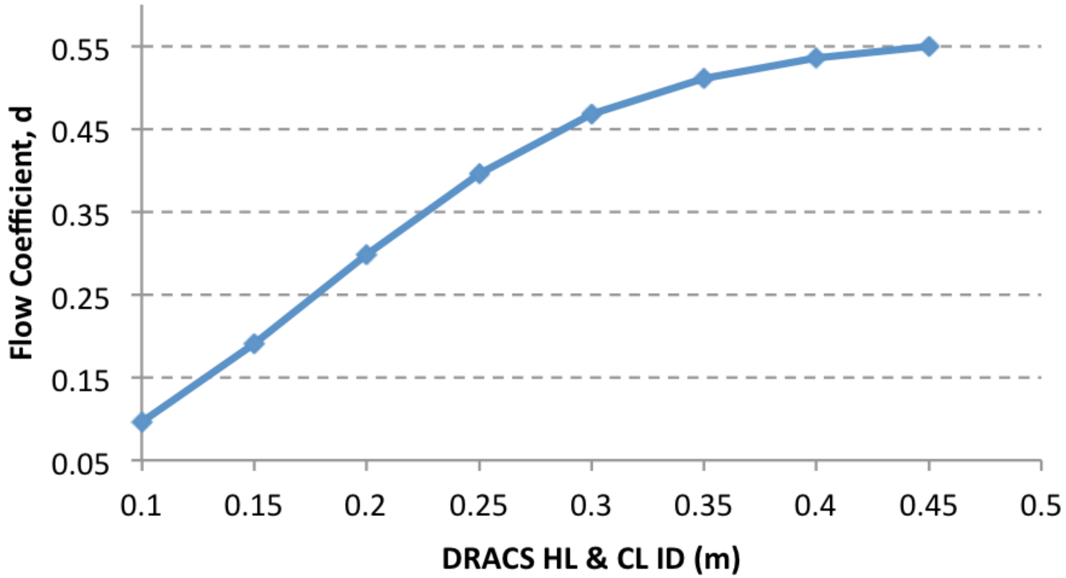


$$\Delta P_f = \Delta P_B$$

$$\dot{m} = \left(\frac{\beta \rho g L_2}{b \bar{c}_P}\right)^{\frac{1}{3-n}} \dot{Q}^{\frac{1}{3-n}} = d\dot{Q}^{\frac{1}{3-n}}$$

Where

$$d = \left(\frac{\beta \rho g L_2}{b \bar{c}_P}\right)^{\frac{1}{3-n}} = flow\ coefficient$$



DAC HT and Pressure Drop Correlations

Heat transfer correlation for finned tube bundle:

$$Nu = 0.192(X_t^*/X_l^*)^{0.2}(S/d_o)^{0.18}\left(e_f/d_o\right)^{-0.14}Re^{0.65}Pr^{0.36}\left(\frac{Pr}{Pr_w}\right)^{0.25} \qquad 100 < Re \leq 2\times10^4$$

$$Nu = 0.0507(X_t^*/X_l^*)^{0.2}(S/d_o)^{0.18}\left(e_f/d_o\right)^{-0.14}Re^{0.8}Pr^{0.36}\left(\frac{Pr}{Pr_w}\right)^{0.25} \qquad 2\times10^4 < Re \leq 2\times10^5$$

$$1.1 < X_t^* < 4.0, \quad 1.03 < X_l^* < 2.5, \quad 0.006 < \frac{S}{d_o} < 0.36, \quad 0.07 < \frac{e_f}{d_o} < 0.715$$

$$Nu = 0.0081(X_t^*/X_l^*)^{0.2}(S/d_o)^{0.18}\left(e_f/d_o\right)^{-0.14}Re^{0.95}Pr^{0.4}\left(\frac{Pr}{Pr_w}\right)^{0.25} \qquad 2\times10^5 < Re \leq 2\times10^6$$

$$2.2 < X_t^* < 4.2, \quad 1.27 < X_l^* < 2.2, \quad 0.125 < \frac{S}{d_o} < 0.28, \quad 0.125 < \frac{e_f}{d_o} < 0.6$$

Pressure drop correlation for finned tube bundle:

$$\Delta P = EuN_r(\rho V_n^2/2)$$

$$Eu = 67.6Re^{-0.7}X_t^{*\,-0.55}X_l^{*\,-0.5}F^{0.5} \qquad 100 < Re \leq 1000$$

$$Eu = 3.2Re^{-0.25}X_t^{*\,-0.55}X_l^{*\,-0.5}F^{0.5} \qquad 1000 < Re \leq 10^5$$

$$Eu = 0.18X_t^{*\,-0.55}X_l^{*\,-0.5}F^{0.5} \qquad 10^5 < Re \leq 1.42\times10^6$$

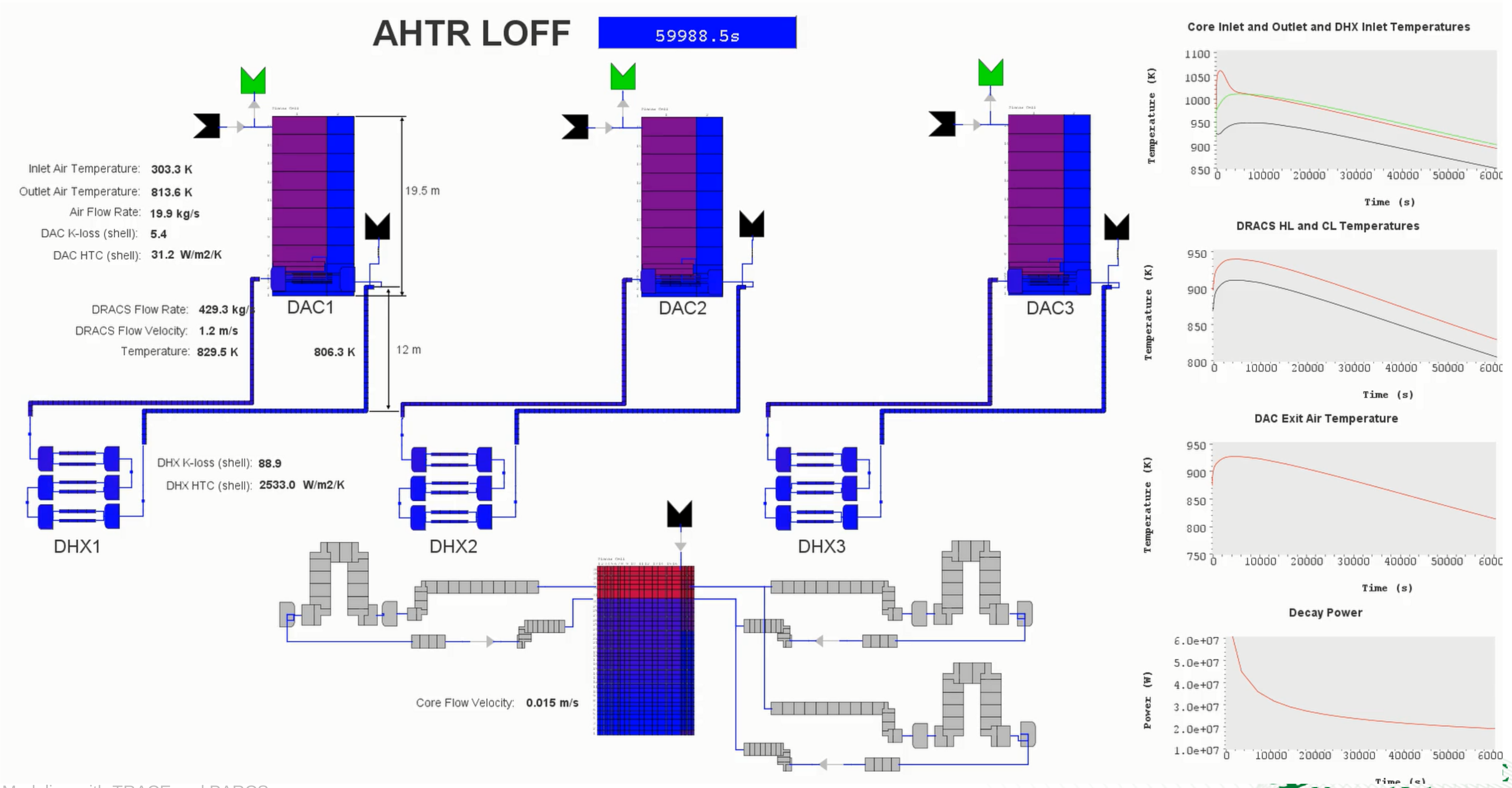
OAK RIDGE National Laboratory

Steady-State Results

Parameter	AHTR Design Values	TRACE
Rated Thermal Power (MWt)	3,400	3,400
Core Flow	28,500	28,500
Relative DHX Shell Side Flow[a]	N/A	3.9%
Core Inlet Temperature (^{o}C)	650	651
Core Outlet Temperature (^{o}C)	700	701
Core Pressure Drop (Pa)	N/A	1.903E+5[b]
DRACS Loop Flow Rate (kg/m^3)	N/A	351
DRACS Hot Leg Temperature (^{o}C)	N/A	620
DRACS Cold Leg Temperature (^{o}C)	N/A	586

Oak Ridge National Laboratory

Loss of Forced Flow (LOFF)



Concluding Remarks

- In the DHX preconceptual design, a fluidic diode is proposed to be installed underneath the DHX to limit the coolant flow through the DHX tubes during normal operation.
- The calculation shows that the reverse flow rate is only about 3.9% of the total core flow rate, and at least for this design, a fluidic diode may not be necessary.
- Additional design trade studies will be needed to confirm this as a general conclusion.
- There is a potential for encapsulating the natural draft heat exchanger during normal operation to prevent tritium escape into the environment.
- Without the encapsulation, the DRACS could be a significant tritium escape route.
- Upper and lower flaps on the heat exchanger would open upon heat up (or loss of power).

Concluding Remarks

- The primary heat exchanger employs a simple tube-and-shell design.
- The primary side of the heat exchanger is FLiBe, and the intermediate side of the heat exchanger is a less expensive salt.
- A preliminary analysis of the PHX design shows that FLiNak performs much better than $KF\text{-}ZrF_4$ as an intermediate coolant in terms of the HX size and the pressure drop through the heat exchanger.
- The FLiBe – FLiNaK HX requires only 60% of the number of tubes required by the FLiBe – $KF\text{-}ZrF_4$ HX, and the pumping power for the FLiBe - FLiNaK HX is only about half that of the FLiBe- $KF\text{-}ZrF_4$ HX.
- However, the $KF\text{-}ZrF_4$ is being considered for the AHTR to avoid the potential expense of inadvertent mixing of lithium isotopes due to a heat exchanger tube leak.

Concluding Remarks

- If the primary coolant system is not pressurized, the primary pumps should be installed on the hot legs instead of on the cold legs because of the significant pressure drop through the primary heat exchangers.
- A sensitivity study was performed to investigate the effect of pump coastdown on core heatup during the LOFF transient.
- It was found that a short period of pump coastdown can effectively reduce the coolant peak temperature at the very beginning of the accident.
- Therefore, a fly-wheel should be considered for the primary and intermediate pumps.

Suggested Studies

- Measurement of thermophysical properties for different salts at different temperatures
  - 15–20% uncertainties in existing experimental data
  - Thermal conductivity data for liquid salts are fragmented and inconsistent, most providing only a single value for thermal conductivity across all temperatures.
  - In particular, almost no measured data are available for thermophysical properties for ZrF_4-containing salts
- Heat transfer and pressure drop experiments for high-temperature fluoride salts under natural and forced convection conditions
  - Experiments would include pipe, narrow rectangular channel, and tube bundle configuration
  - Measurement of the heat transfer of salts at moderate Re would be very useful since fluoride salt-cooled reactors typically operate with Reynolds numbers below 10,000 in the reactor core
  - However, existing empirical heat transfer models have large discrepancies at relatively low Re

Suggested Studies

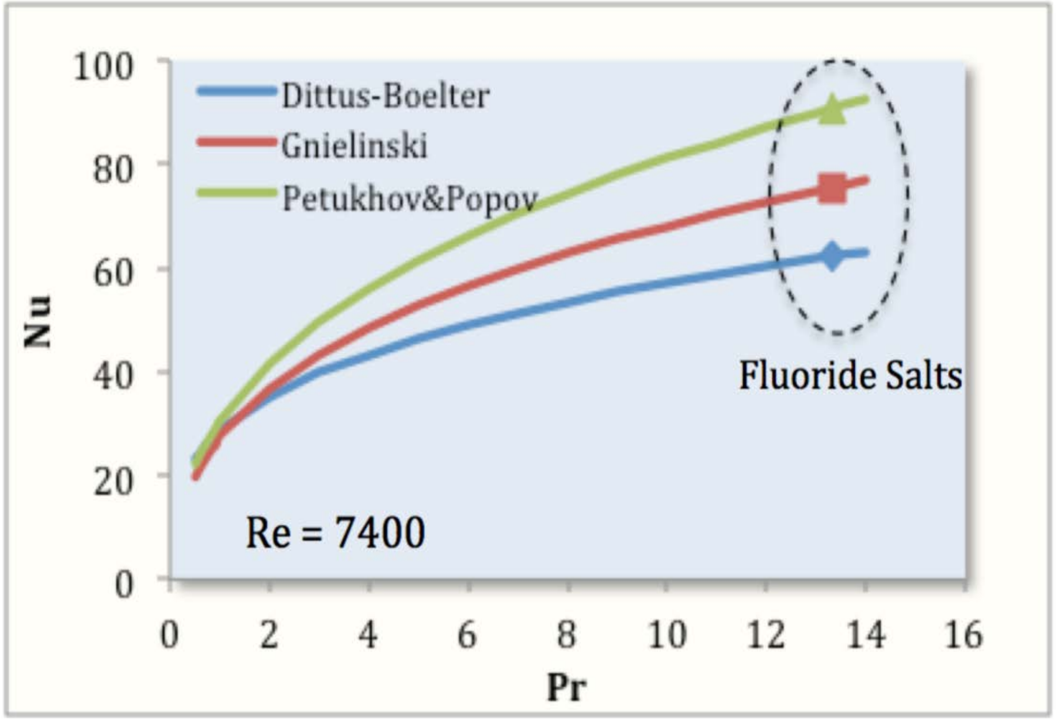
- Model development for heat transfer and pressure drop for geometries and fluids with a wider range of applicability
  - Development of accurate empirical correlations of heat transfer and pressure drop are extremely important for forced convective flow with moderate Re (< 10,000) and natural convection flow
  - Correlations of heat transfer and pressure drop for the HX shell side cross flow should be further investigated
  - Experimentation may be needed for a specific HX design
- CFD analysis
  - Thermal mixing and flow stratification in the core upper plenum following a reactor scram is recommended
  - This may have a profound impact on natural circulation flow and therefore decay heat removal

Questions?

Extra Slides

Concluding Remarks

- The accuracy of the heat transfer analysis depends on the accuracy of the properties of the salt being analyzed.
- Many of the salts have limited amounts of thermophysical property data available, and additional work needs to be done to measure the thermophysical properties of fluoride salts of interest. This is especially true for the less common salts such as Zr salts.
- The correlations of heat transfer and pressure drop for the HX shell side cross flow should be further investigated.
- Experimentation may be needed for a specific HX design.



Modelling of Advanced Reactor Concepts at CNL

Alex Levinsky (CNL)

Modeling of Advanced Reactor Concepts at CNL

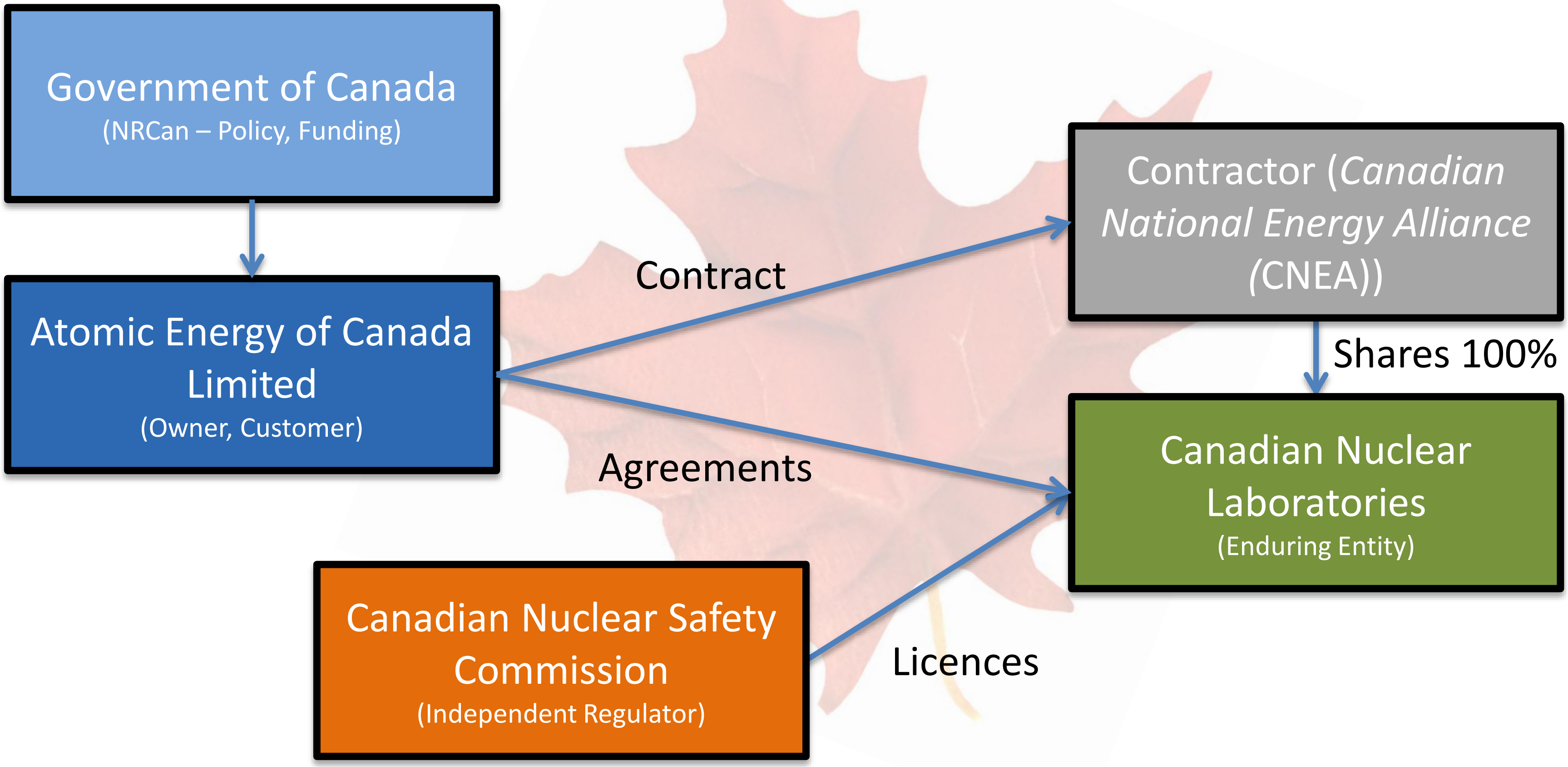
Workshop on Tools for Modeling and Simulation of Fluoride Cooled High Temperature Reactors (FHR) – Gaps and Development Needs, Atlanta, GA, USA

Dr. A. Levinsky

Outline

- Canadian Nuclear Laboratories – structure and missions
- Modeling of advanced reactors –current state
- Applicability of the used modeling tools to FHRs and challenges
- Coupled simulations of transients in advanced reactors – future work
- Modeling Needs for Performing Code Coupled Calculations and Transient Analysis of FHRs
- Summary

CNL: Roles & Relationships at GoCo End-State



CNL's Missions

- Provide the sustainable energy solutions including the extension of the reactor operating lifetimes, hydrogen energy technologies, fuel development, advanced reactors and SMRs.
- Support radiochemical therapies.
- Enhance national and global nuclear safety and security.
- Develop decommissioning technologies.

Modeling of Advanced Reactors - Current State

Motivation

- There is an interest in using small reactors in Canada: Saskatchewan province and Northern provinces and territories;
- Most of the proposed SMR designs are based on the advanced technologies - molten-salt, gas-, lead-, and sodium-cooled concepts.
- These concepts should be evaluated in order to chose the most appropriate ones from the technical and economical points of view.
- The evaluation requires adequate simulation tools.

Modeling of Advanced Reactors - Current State

Focus of the Work in the last 2 Years

- Development of the reactor physics models for gas-cooled, molten-salt and liquid-metal-cooled concepts.
- Parametric study - reactor size, power, fuel enrichment, burnable poison concentration, control rod configuration etc.
- Burnup calculations – length of the fuel cycle as a function of fuel enrichment, core size, power etc.
- Assessment of the nuclear data impact on the reactor safety parameters.
- Transient analysis.
- Development of the thermal hydraulics models.

Modeling of Advanced Reactors - Current State

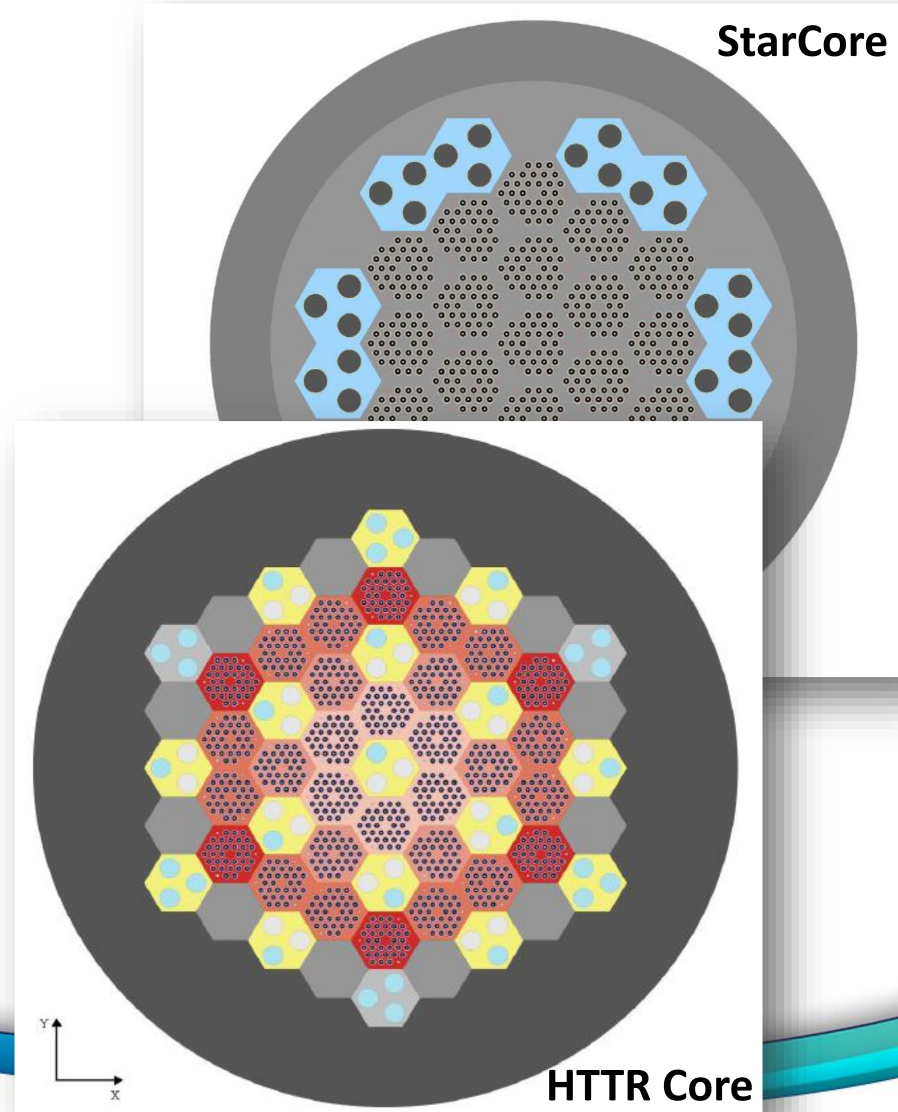
Gas-Cooled Reactors (1)

Concepts:

- ❑ Pebble bed type reactor – StarCore concept[1]
- ❑ Prismatic reactor - High Temperature engineering Test Reactor (HTTR)[2]

Specifics:

- ❑ TRISO fuel
- ❑ Graphite moderator
- ❑ Thermal spectrum



Modeling of Advanced Reactors - Current State

Gas-Cooled Reactors (2)

Reactor Physics:

- Modeling tools: SERPENT2 – a Monte Carlo neutronic code developed at the VTT (Technical Research Center in Finland).
- Advantages of the tools: burnup calculations and four options are available for modeling of TRISO-based fuels.

Thermal hydraulics:

- Modeling tools: CATHENA - Canadian Algorithm for THErmal hydraulic Network Analysis transient.
- CATHENA has been traditionally used for the modeling of CANDU reactors (pressurised heavy water reactors with horizontal pressure tubes containing fuel bundles, and moderator and coolant physically separated from each other), but this code is very flexible in terms of creation of the thermal hydraulics network elements.
- The physical properties of helium and graphite are built-in the code.

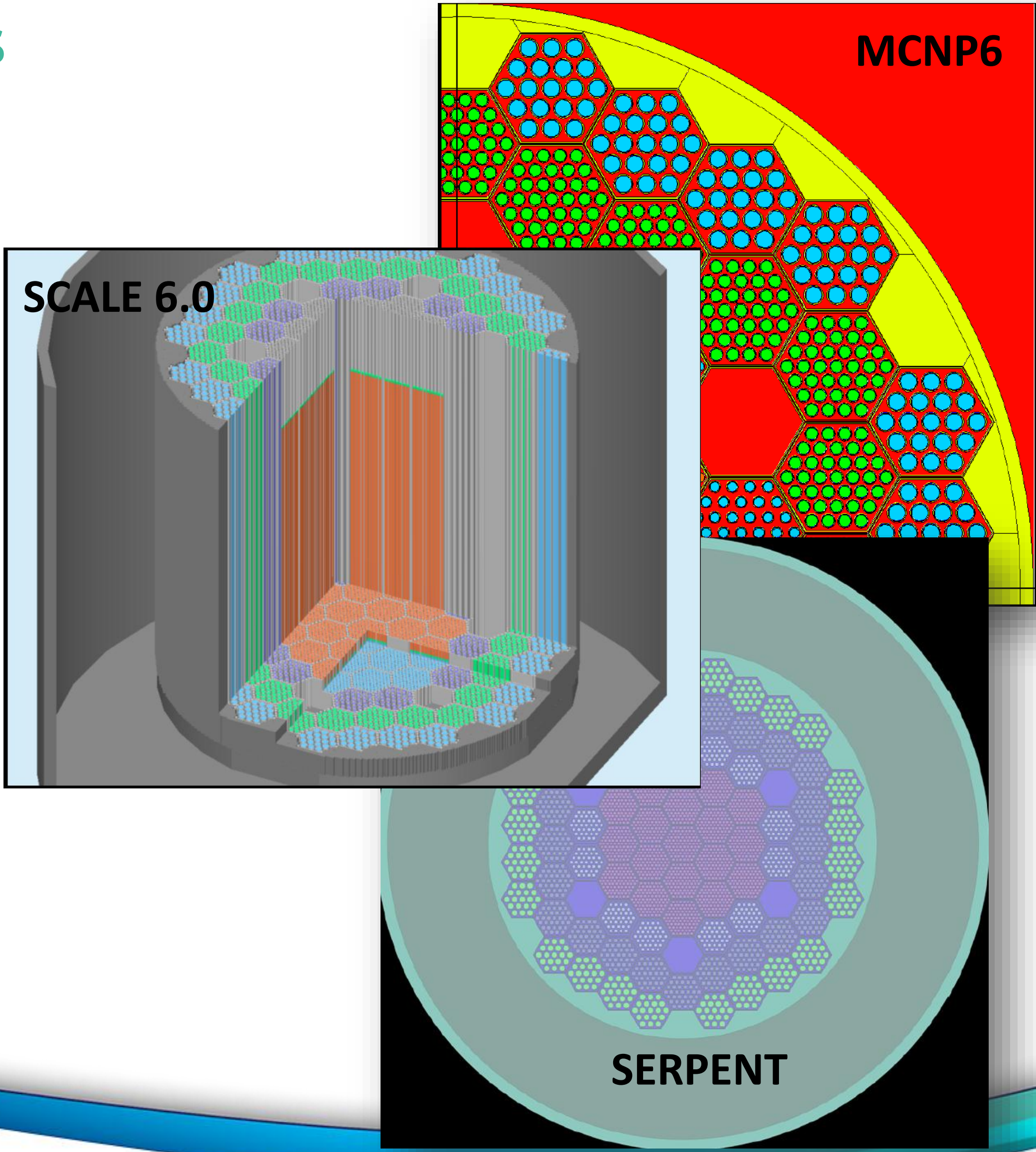
Modeling of Advanced Reactors – Current State

Liquid-metal-cooled Concepts

Concept: SEALER -SwEdish Advanced LEad Reactor)[3]

Specifics:

- Fast spectrum
- Commercially available standard fuel;
- UO_2 with 19.9% enrichment;
- Design thermal power: from 10 to 30 MWth;
- Core life: between 10 and 30 full power years (at 90% availability) ;
- A maximum temperature of the lead coolant below 450°C;



Modeling of Advanced Reactors - Current State

Liquid-metal-cooled Concepts

Reactor Physics Modeling tools:

- SERPENT2.1.26
- SCALE6 and TSUNAMI module
- MCNP6
- Deterministic codes developed at the Polytechnique Montréal:
  - Dragon5 – a lattice physics code.
  - Donjon5 – a reactor physics code.

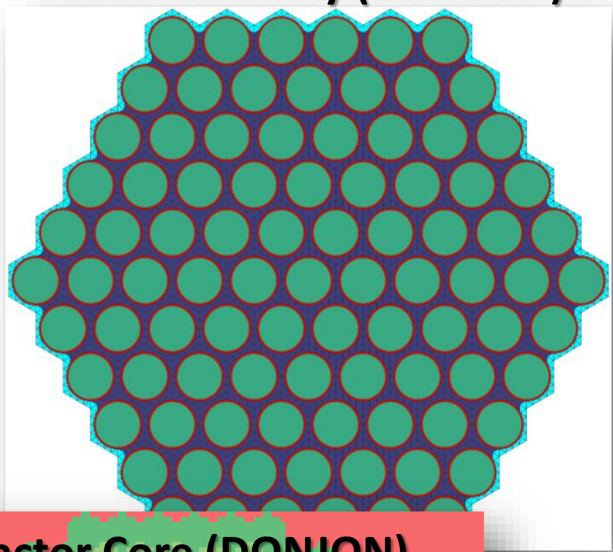
Advantages of the tools:

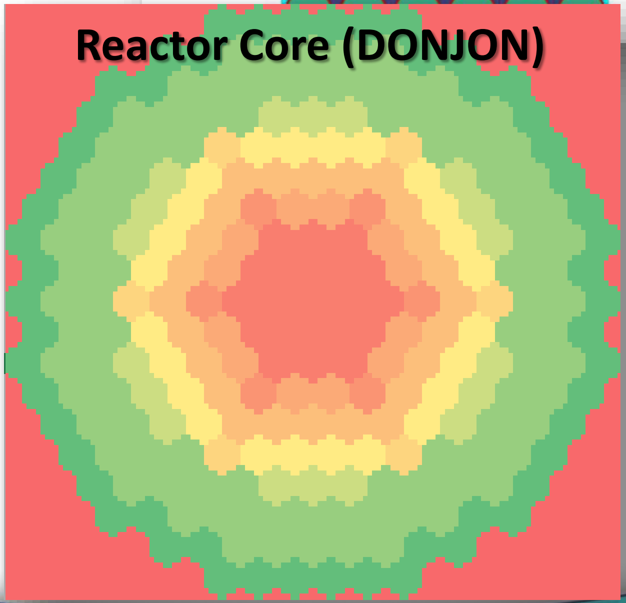
- Availability of the hexagonal geometry, uncertainty analysis tools, burnup calculations, time dependent simulations.

Other modeling tools:

- NJOY and Dakota

Fuel Assembly (DRAGON)





Modeling of Advanced Reactors - Current State

Molten-Salt Reactors

Concepts:

- Integral Molten Salt Reactor(IMSR) – Terrestrial Energy design[4]
- Molten-Salt Reactor Experiment (MSRE)[5]

Specifics:

- Liquid fuel
- Graphite moderator
- Flowing fuel involving drift of delayed neutron precursors
- Continuous addition and removal of fuel

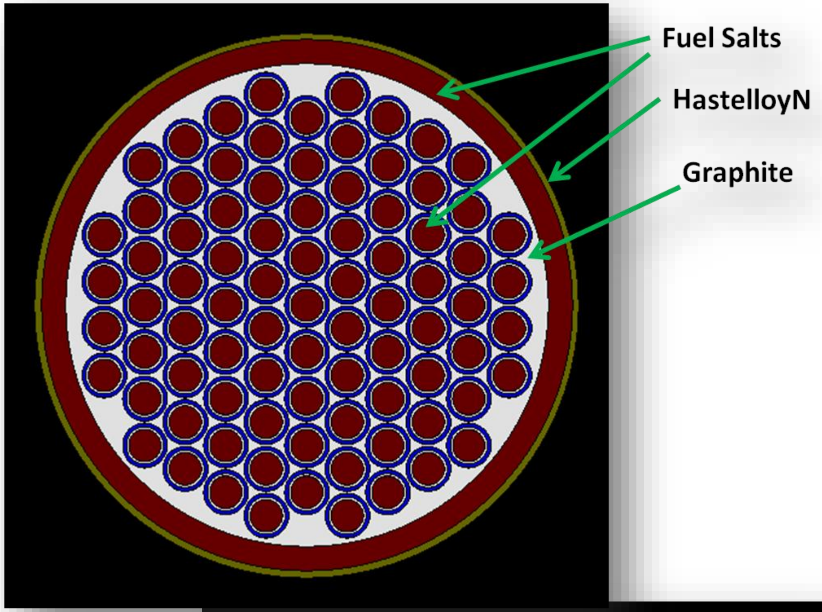
Reactor Physics Modeling tools:

- SERPENT2.1.26

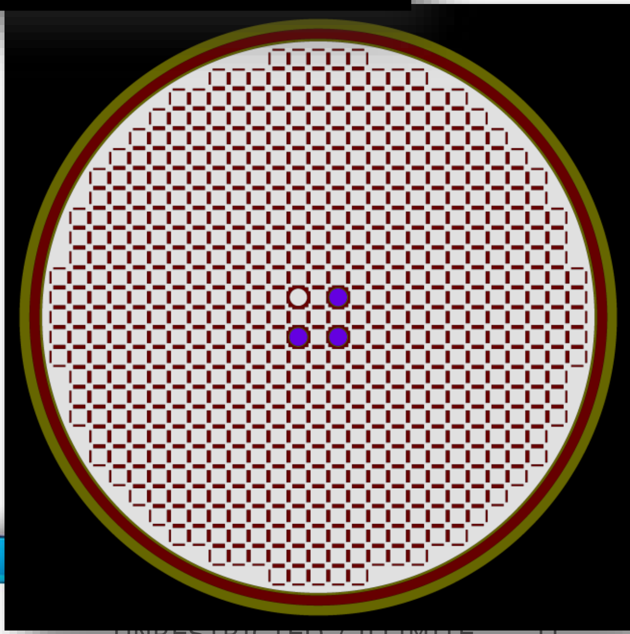
Advantages of the tools:

Transfer rates of nuclides or elements between materials, reprocessing and depletion schemes can be defined.

IMSR



MSRE



Applicability of the used Modeling Tools to FHRs and Challenges

FHRs specifics

FHRs have not been modeled but the modeled reactor concepts have the features relevant to the FHRs:

- TRISO fuel,
- Prismatic fuel assembly,
- Pebble bed structure,
- Graphite blocks,
- Burnable poison,
- Specific material properties,
- Specific thermal hydraulics,
- Specific fuel performance,
- Flowing fuel involving drift of delayed neutron precursors,
- Transit time of the fuel through the core components.

Applicability of the used Modeling Tools to FHRs and Challenges

Code requirements

Identified functional requirements:

- ❑ Reactor Physics and lattice physics codes:
  - TRISO fuel,
  - Hexagonal geometry,
  - Flowing fuel involving drift of delayed neutron precursors,
  - Continuous addition and removal of fuel,
  - Flexibility in using of different nuclear data,
  - Burnup and fuel cycle analysis,
  - Estimation of radiation emission of the reactor components and decay power.
- ❑ Thermal hydraulics codes:
  - Material properties
  - Appropriate component models
  - Validation data

Coupled Simulations of Transients in Advanced Reactors - Future Work

"Prototype coupled toolset for modeling SMR transients" project starting from April of 2017

- The objectives of these three year project are:
  - To create a toolset providing capabilities to model coupled thermal hydraulics/reactor physics simulations of transients in SMRs based on advanced concepts.
  - To demonstrate the coupled toolset capabilities in transient modeling
  - To build capabilities in performing CFD modeling of the transients in SMRs based on advanced concepts.
- The advanced reactor concepts proposed for the project are: liquid-metal-cooled, gas-cooled, molten-salt and fluoride-cooled.
- Likely that the coupled toolset will not be applicable to all concepts.

Coupled Simulations of Transients in Advanced Reactors - Future Work

Reactor Physics/Lattice Physics Codes

Proposed simulation tools: SERPENT2, SCALE6.2, PARCS , DIF3D/VARIANT, MPACT,..?

Planned work:

- Evaluation of the selected codes. A reactor physics code must have a time-dependent capability.
- Testing of appropriate nuclear data.
- Modeling of steady-state and transients without coupling to thermal hydraulics.
- Evaluation of the code performance and results.
- Performing TH/reactor physics coupled simulations for selected concepts and transients.

Coupled Simulations of Transients in Advanced Reactors - Future Work

Thermal Hydraulics Tools

Proposed simulation tools: RELAP5-3D, TRACE, ..?

Planned work:

- Evaluation of the selected codes.
- Search of the experimental/benchmark data.
- Implementation of models/properties if required.
- Modeling of steady-state and transients without coupling to reactor physics.
- Evaluation of the code performance and results.
- Performing TH/reactor physics coupled simulations for selected concepts and transients.

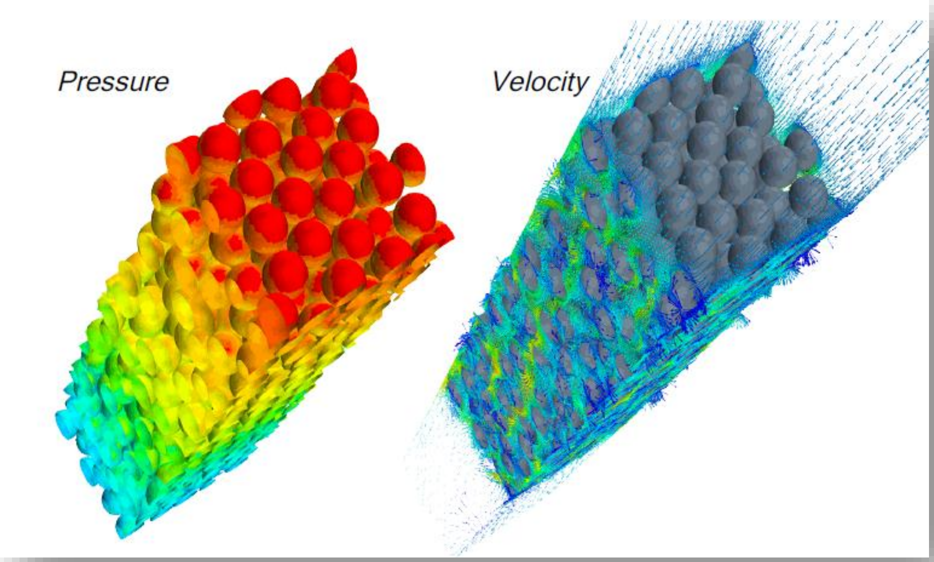
Coupled Simulations of Transients in Advanced Reactors - Future Work

CFD Tools

Proposed simulation tools: STAR-CCM+

Planned work:

- Identification of the gaps involved in the use of STAR-CCM+ for modeling of advanced reactor concepts
- Incorporation of the material properties into the code.
- Development of the suitable turbulence models.
- Performing steady-state, short-transient, and code-coupled (STAR-CCM+/RELAP5-3D) simulations.



Pressure and flow distributions in a pebble bed modular reactor[6]

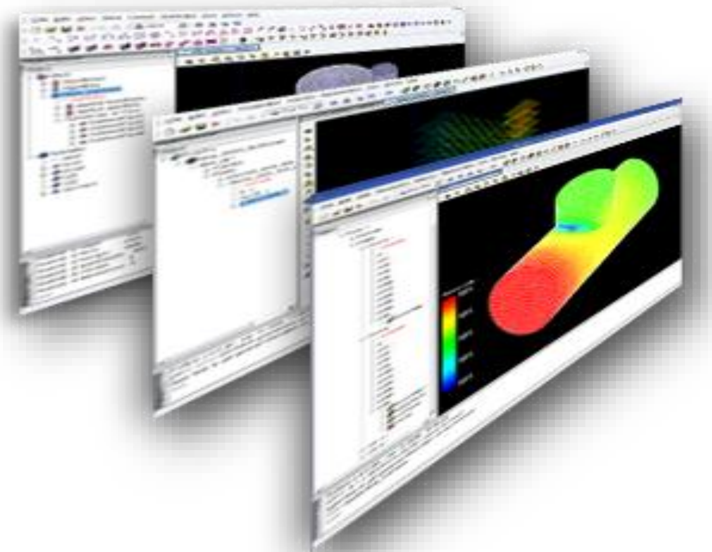
Coupled Simulations of Transients in Advanced Reactors - Future Work

Platform/Methods for Performing Coupled Calculations

The two possible candidates are:

- SALOME - an open source integration platform for numerical simulation, which is being developed since 2001 by CEA, EDF and OPEN CASCADES[7].
  - Supports interoperability between CAD modeling and computation software.
  - Provides platform for coupling, hosting, integration, execution of the computation codes and post-processing of the results.

  It is used by CNL for the PHWR coupled calculations with the NESTLE-C, SERPENT, CATHENA, and BISON codes.
- VERA - the Virtual Environment for Reactor Applications components[8].



Examples of simulations performed using SALOME[7]

Modeling Needs for Performing Code Coupled Calculations and Transient Analysis of FHRs

- General:
  - Identification of normal operation conditions and accident scenarios,
  - Estimation of the source term,
  - Validation data.
- Reactor Physics Codes:
  - Time dependent capability,
  - Capability to model movement of a control rod.
- Thermal hydraulics and CFD Codes:
  - Material properties,
  - Component models,
  - Models capturing relevant physical phenomena.

Summary

- CNL has been working on the development of capabilities in modeling of advanced reactors – gas-cooled, liquid-metal-cooled, molten-salt and fluoride-cooled.
- The key areas of interest are the following:
  - Implementation of the material properties in thermal hydraulics codes, if required.
  - Comparison with the experimental/benchmark data, if possible.
  - Performing time dependent simulations.
  - Performing reactor physics/thermal hydraulics coupled transient simulations.
  - Implementation of material properties and turbulent models in the CFD code.
  - Performing thermal hydraulics/CFD coupled simulations.

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Thank you!

Technical lead: Alex Levinsky

Team members: Fred P. Adams, Nicholas Chornoboy, Blair Bromley, Tariq Jafri, Sourena Golesorkhi, Alex Trottier, Dan Roubtsov, Geoff Waddington, Geoff Edwards and Daniel Wojtaszek

Canadian Nuclear Laboratories | Laboratoires Nucléaires Canadiens

COMET tool set

Farzad Rahnema (GT)

Coarse Mesh Transport (COMET) Toolset

Farzad Rahnema
Computational Reactor and Medical Physics Lab (CRMP)
Georgia Institute of Technology

Atlanta, GA, USA
March 8 – 9, 2017

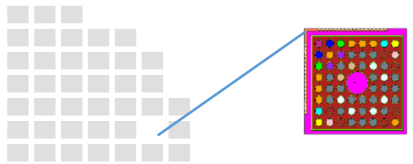
Outline

- COMET method
- Numerical verification of COMET
- Application of COMET beyond reactors
- Recent capability extensions
- Coupled thermal fluid/neutronics COMET results
- Potential issues for FHR application
- Future work
- Acknowledgement

COMET, a hybrid stochastic deterministic transport method

Based on incident flux response expansion theory

- Decompose the core problem into a set of local fixed source problems over non-overlapping coarse meshes



- **Stochastic transport** is used as the local solver for each unique mesh using a set of known basis functions (BF) – i.e., the unknown incident flux is expanded in phase space using the same BF
- Use superposition of RFs to calculate outgoing fluxes given incident fluxes on the mesh boundary
- Sweep through the core using **deterministic transport** until k-eff and incident fluxes are converged

COMET method – core calculation

- Solve the transport equation with arbitrary BC

$$H\psi(\vec{r},\hat{\Omega},E)=\frac{1}{k}F\psi(\vec{r},\hat{\Omega},E)\ +\ \text{external source } (k=1) + \text{external } BC$$

Where,

$$H\psi(\vec{r},\hat{\Omega},E)\equiv$$

$$\hat{\Omega}\cdot\vec{\nabla}\psi+\sigma_t(\vec{r},E)\psi-\int_0^{\infty}\int_{4\pi}\sigma_s(\vec{r},\hat{\Omega}',E'\rightarrow\hat{\Omega},E)\psi(\vec{r},\hat{\Omega}',E')d\hat{\Omega}'dE',$$

$$F\psi(\vec{r},\hat{\Omega},E)\equiv\frac{\chi(\vec{r},E)}{4\pi}\int_0^{\infty}\nu\sigma_f(\vec{r},E')\int_{4\pi}\psi(\vec{r},\hat{\Omega}',E')d\hat{\Omega}'dE',$$

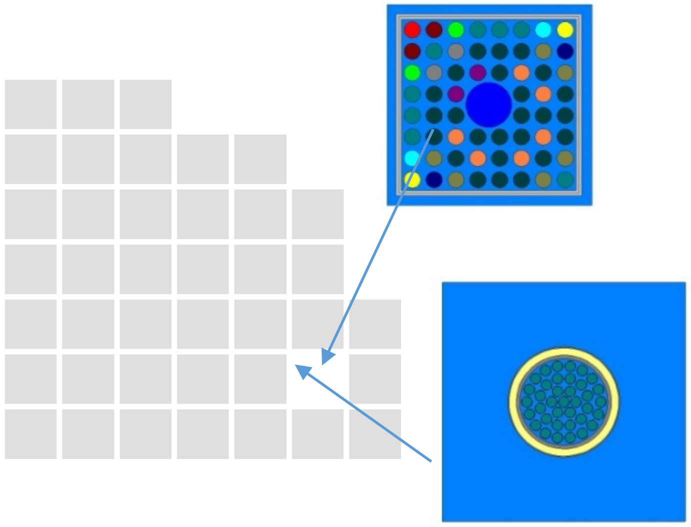
Method – domain decomposition

- Decompose the global problem as a set of local fixed source problems over non-overlapping coarse meshes V_i

$$H\varphi(w_i) = \frac{1}{k} F\varphi(w_i)$$

$$\text{with} \quad \varphi(w_i^-) = \psi(w_i^-),$$

$$\text{for } \vec{r} \in \partial V_i,$$



- If ψ is the solution to the TE for the whole core problem, then $\varphi(w_i) = \psi(w_i) \text{ in } V_i,$

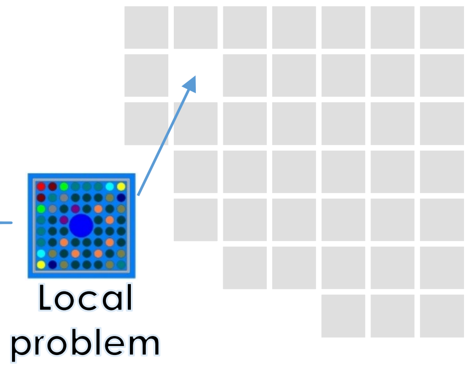
Incident flux expansion method

- Expand the angular flux at mesh boundaries using pre-computed local solutions as expansion functions

$$\psi_i(\vec{r},\hat{\Omega},E)=\sum_{m=0}^{\infty}\sum_{s}c_{is}^{m}R_{is}^{m}(\vec{r},\hat{\Omega},E),\qquad c_{is}^{m}=\int dw_{is}^{-}\gamma(w_{is}^{-})\Gamma^{m},$$

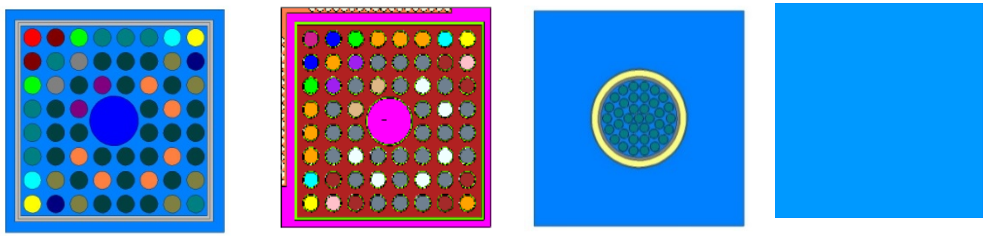
$$HR_{is}^{m}(w_i)=\frac{1}{k}FR_{is}^{m}(w_i)$$

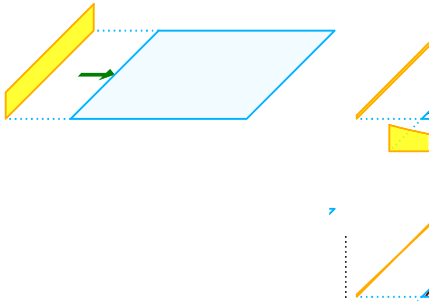
$$\textit{with}\quad R_{is}^{m}(w_{is}^{-})=\begin{cases}\Gamma^{m}(w_{is}^{-}), & \text{for } \vec{r}\in\partial V_{is}\\ 0, & \text{otherwise}\end{cases}$$



$$\Gamma^{m,n,p,q,g}(x,y,\mu,\phi)=f_g P_m(x)P_n(y)P_p(\phi)P_q(\mu)$$

Surface-to-surface/volume response functions for unique meshes





Γ^m

R_{is}^m

Iteration method

- The RF library (a set of response functions) is precomputed for a chosen core *k-eff* (=1, e.g.) using a **stochastic transport solver**

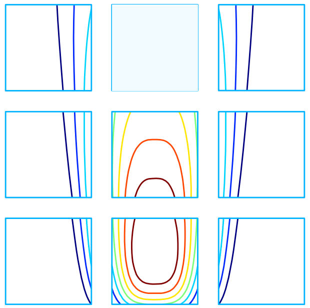
- Inner iteration on incident angular flux
  - Start from any mesh and use an initial guess of *k* and incident fluxes
  - Compute outgoing fluxes
  - Sweep through the core

$$\varphi^{+}_{m,s} = \sum_{m',s'} R^{m'\to m}_{s'\to s}\,\varphi^{-}_{m',s'}$$

- Outer iteration on *k*
  - Estimate *k* as

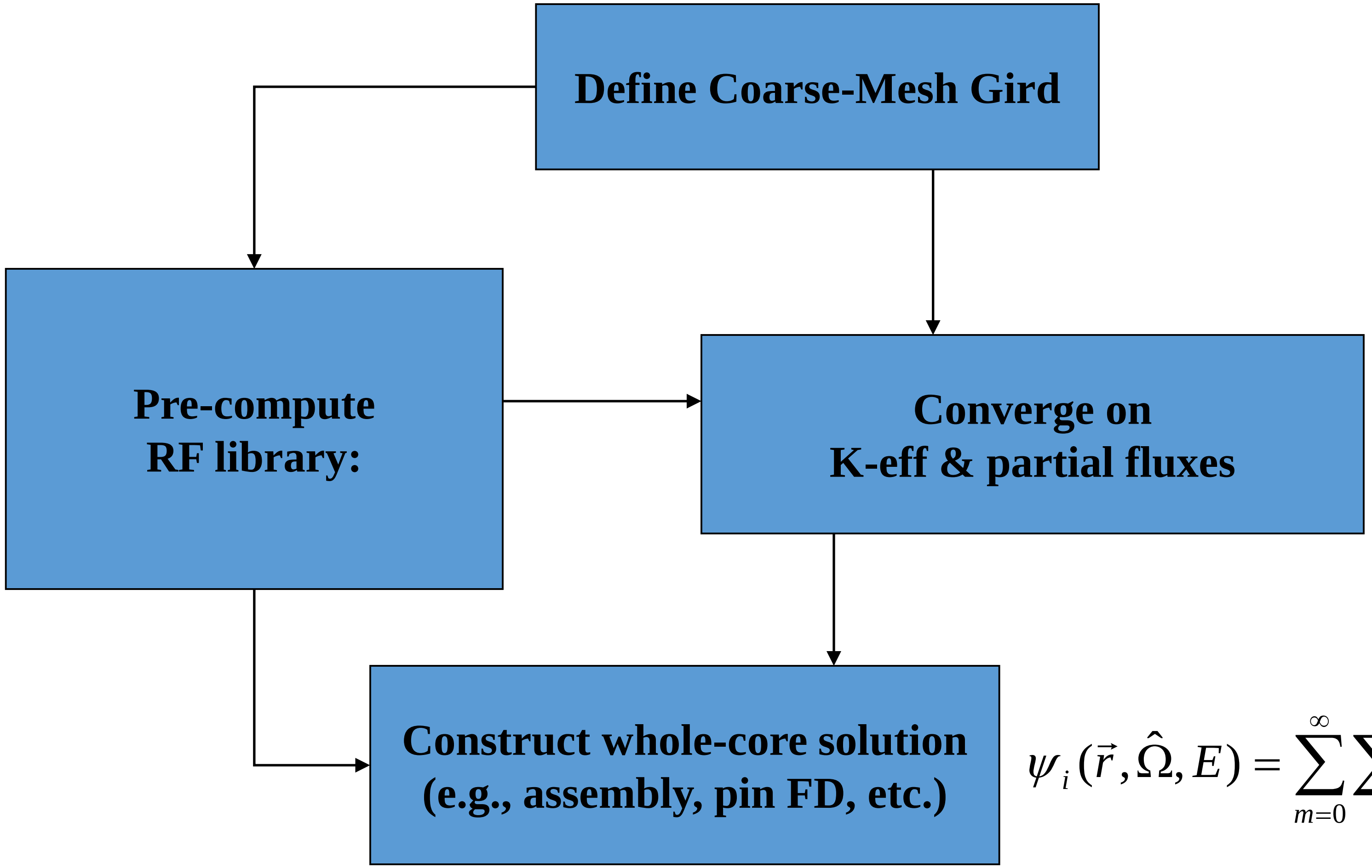
$$k^{(u)} = \frac{\int d\mathbf{w}\ \mathbf{F}\varphi^{(u)}}{L + \int d\mathbf{w}\ \mathbf{A}\varphi^{(u)}}$$

  - Update RFs for new k



- Repeat until convergence

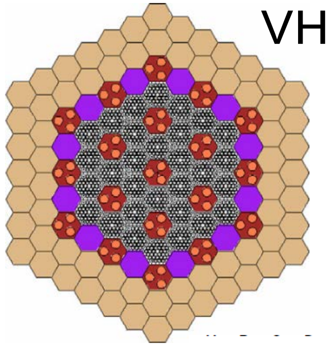
COMET Flowchart



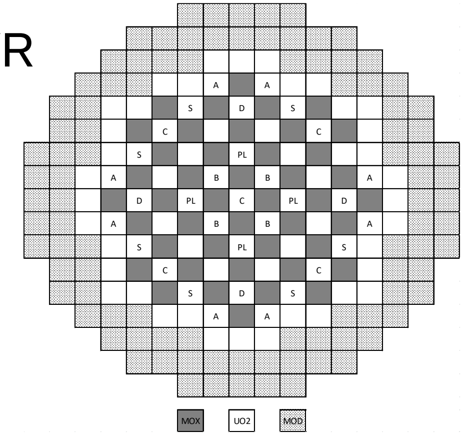
$$\psi_i(\vec{r},\hat{\Omega},E)=\sum_{m=0}^{\infty}\sum_{s}c_{is}^{m}R_{is}^{m}(\vec{r},\hat{\Omega},E),$$

SS whole-core benchmarks

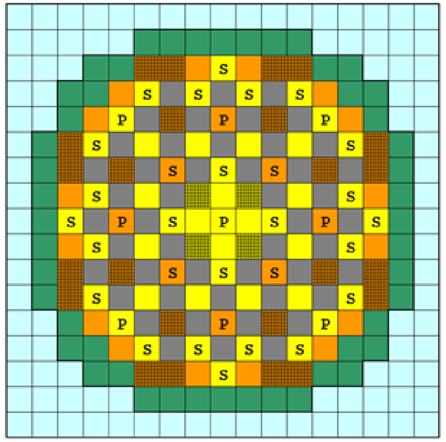
VHTR & HTTR



MOX-PWR

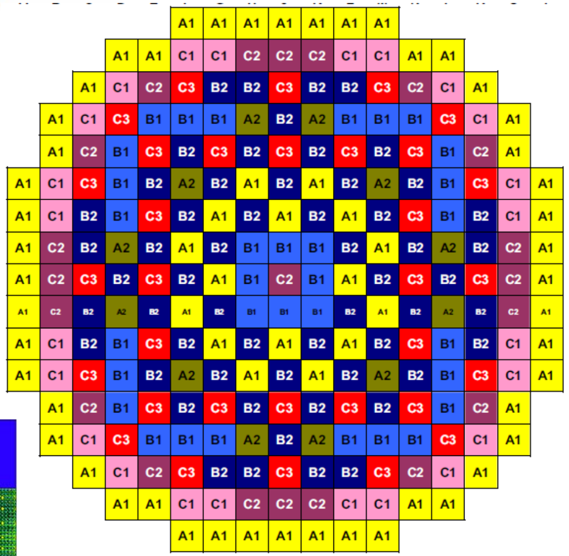


PWR w/Gd

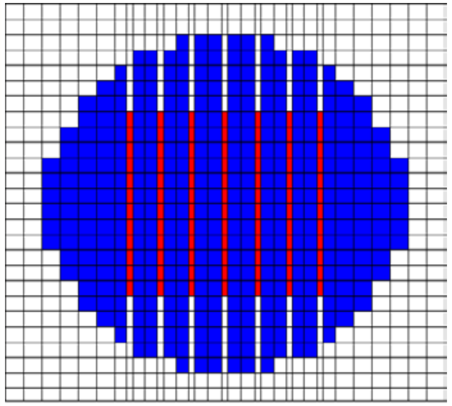


Assembly Type	
	Moderator
	Fresh
	15 GWd/T
	35 GWd/T
	50 GWd/T
	Gadded Fuel Assembly
S	Control Rod Location
P	Power Shaping Control Rod Location

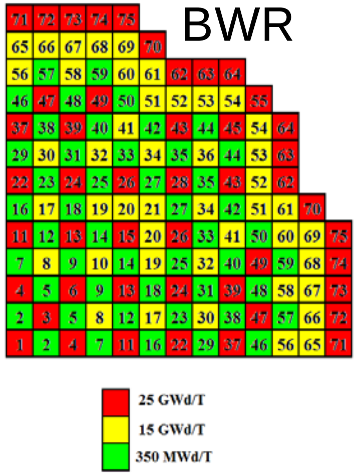
EPR



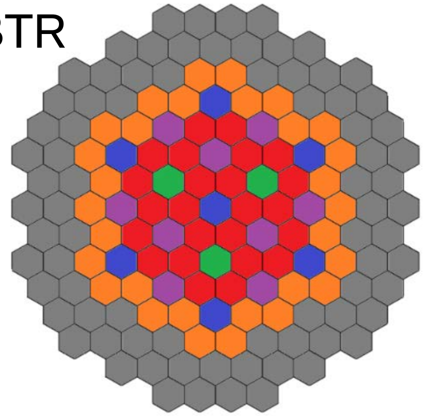
CANDU6



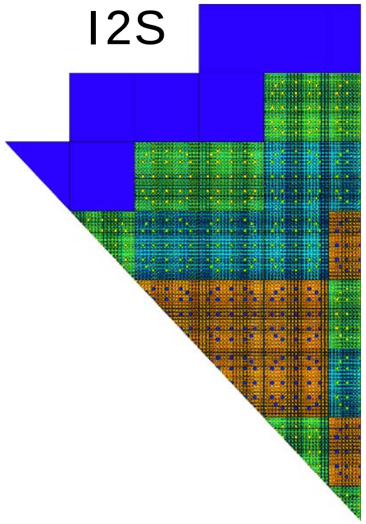
BWR



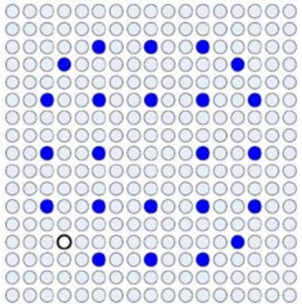
ABTR



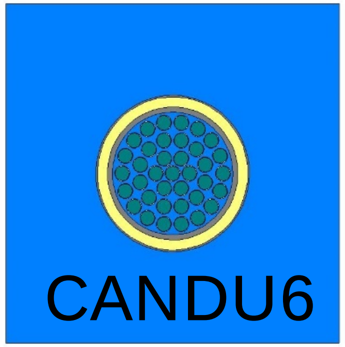
I2S

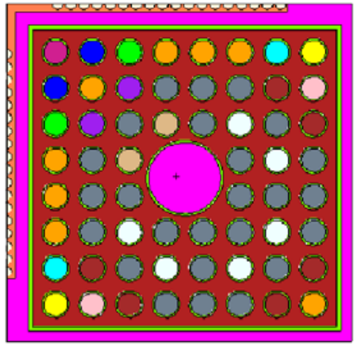


Benchmark Assembly/Blocks/Bundles

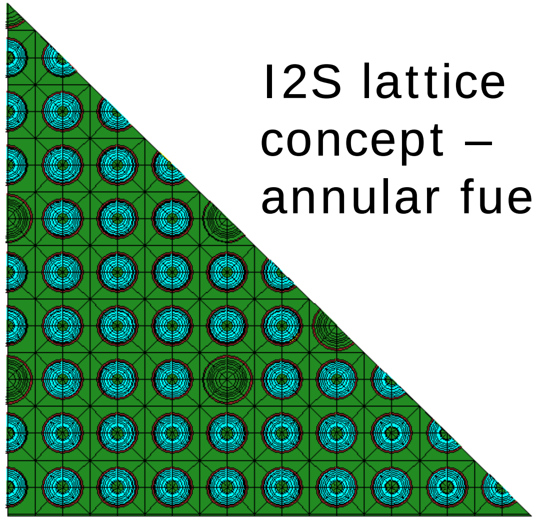


EPR

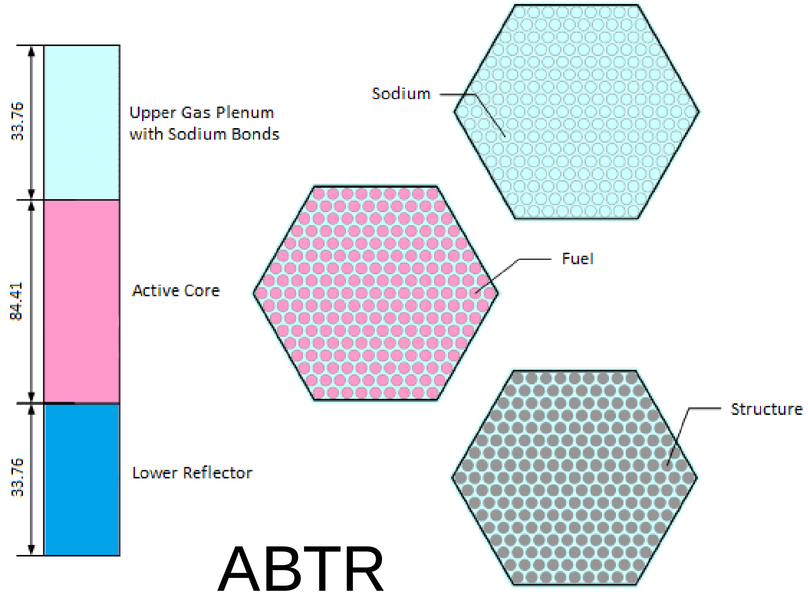




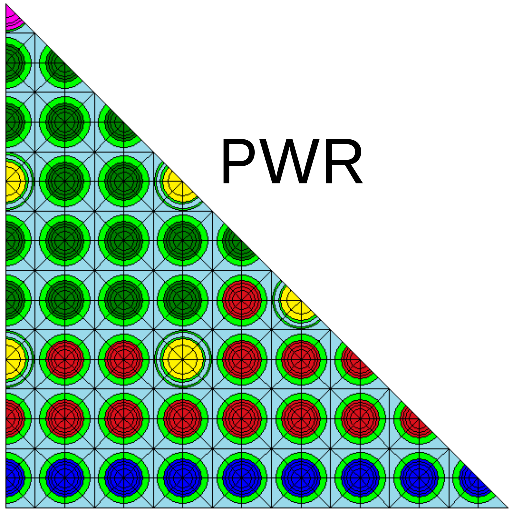
BWR

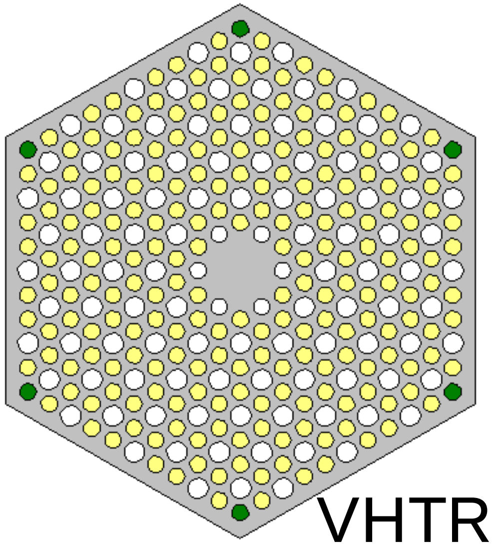


I2S lattice concept – annular fuel



ABTR





VHTR

COMET benchmarked against Monte Carlo

- Benchmark problems: whole-core CANDU6, BWR, PWR (MOX, Gadded, EPR, I2S), ABTR, VHTR, HHTR (coupled neutronics & thermal hydraulic), and C5G7
- Eigenvalue & pin + assembly averaged fission density results agree with Monte Carlo very well
  - Monte Carlo has issue with solution convergence in large whole-core problems
- COMET computational speed is 3-4 orders of magnitude faster than MCNP

Other Applications - coupled (e, γ) transport

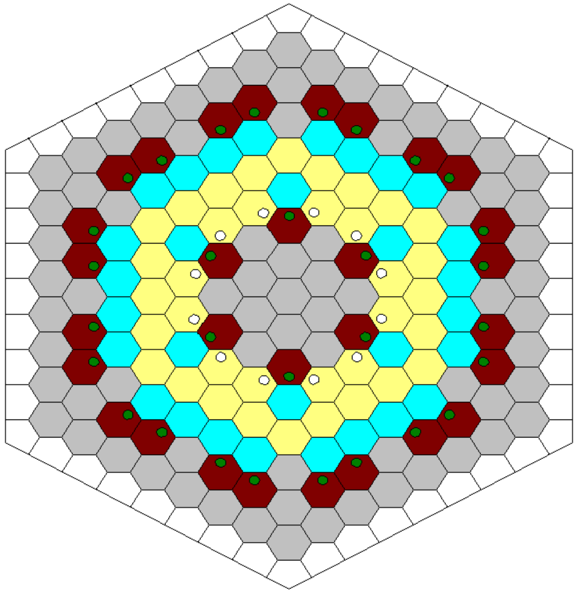
- Medical physics
  - Radiotherapy Calculations in 3D phantoms with an arbitrary source
- Nucelar security
  - On-the-fly calculation of radiation sensors for SNM detection

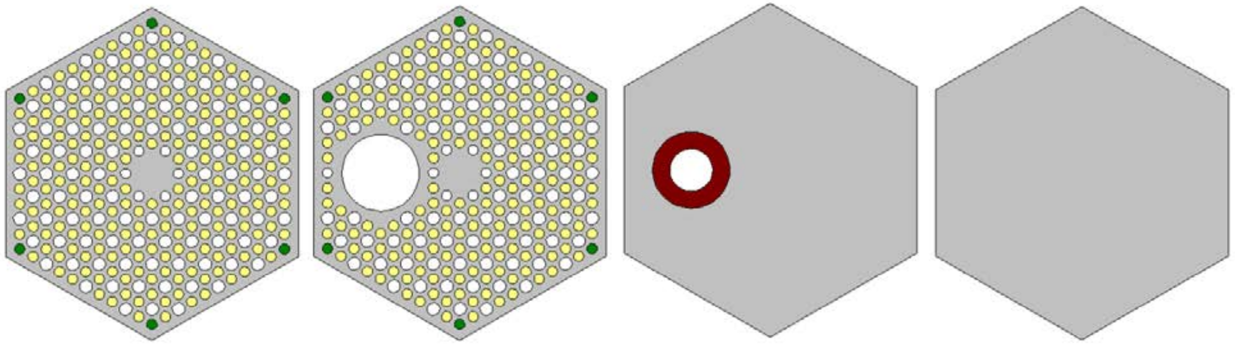
Recent extensions of capability

- Coupled neutronics-thermal hydraulic COMET method for prismatic HTGRs
  - SS-TH parameters calculated using a 3-D unit cell based thermal-fluids solver
- The Stochastic Particle Response Calculator (SPaRC)
  - Allows for efficient generation of response functions using Monte Carlo
  - Can be used for on-the-fly RF generation
- The Application Programming Interface for Depletion Analysis (APIDA)
  - Highly efficient portable burnup solver for in-memory implementation
  - Uses both Chebyshev Rational Approximation Method (CRAM) and a linear chain method
- Further computational efficiency gains enabling on-the-fly response generation and depletion by
  - adaptive flux expansion method
  - parallel computing
- Adjoint capability (no adjoint RF library needed)

Coupled thermal fluid/neutronics COMET Results – VHTR in 3D

- Core & assembly layout





Parameter	Value	
Thermal Power	350	MW
Inlet Temperature	259	^{o}C
Inlet Pressure	6.39	MPa
Mass Flow Rate	157.1	kg/s

- Fuel T range: 350, 537.5, 725, 912.5, and 1100
- Other material T range: 300, 475, 650, 825, and 1000 C

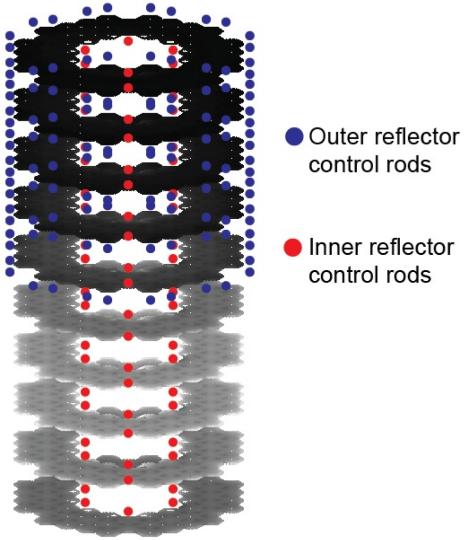
Results – VHTR, near critical condition k=0.99758 ± 100 pcm

Computational Time per Iteration

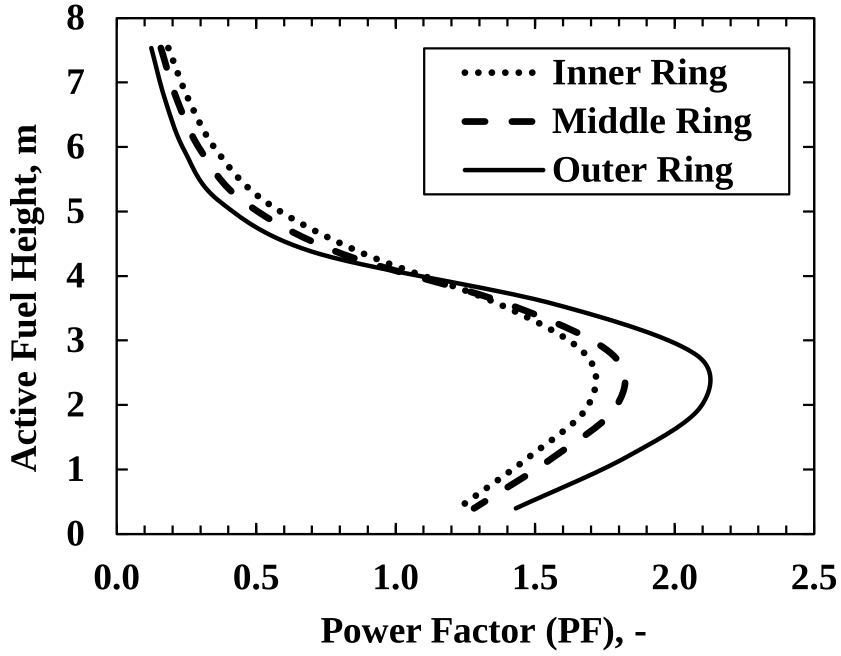
TH#	COMET #	TH Time (hr)	COMET Time (hr)
-	1	-	0.46
1	2	18.22	1.05
2	3	20.11	1.25
3	4	20.09	1.03
4	5	18.31	1.02
5	-	19.79	-
TOTAL		96.52	4.81

Near-Critical Configuration Core T

Material	Peak, °C	Average, °C
Fuel	1024	562
Graphite	845	339
Coolant	806	689

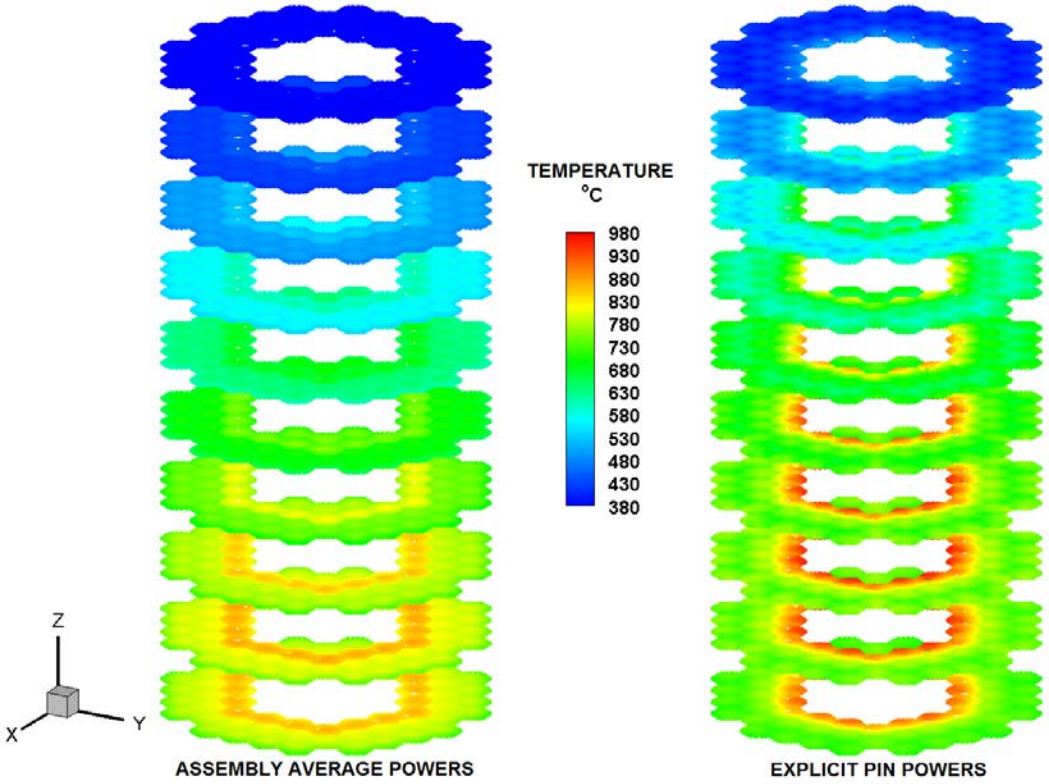


Optimal critical control rod configuration



Importance of pin resolved power

- ARO 3-D fuel temperature distribution comparison



- Peak fuel T is 85°C cooler than the explicit pin power case
- Peak graphite and coolant temperatures are also underestimated

Issues for FHR application

- Issue: Currently, based on multigroup theory - same cross section issues as other transport codes
- Resolution: extension to continuous energy

Add-on features/options under development:

- time dependent COMET
- Implementing the new APIDA module for in-memory depletion in COMET
- Using SPaRC as a standalone and on-the-fly stochastic RF generator for COMET instead of the modified MCNP

Future Work

- Continuous-energy COMET
- Validation
- Lattice depletion code: COMET + APIDA +SPaRC
- Whole-core depletion: COMET + APIDA +SPaRC
- Couple to other physics
  - E.g., CFD/TH, materials, graphite dimensionality changes
  - Next steps: CFD coupling for FHR, MSR
- Uncertainty Quantification
- Online simulation/monitoring by adapting to instrument reading

Acknowledgement

- Contributors (Georgia Tech, CRMP):
  - Many graduate students through PhD theses
  - Faculty: Srinivas Garimella (thermal hydraulics for VHTR), Dingkang Zhang
- Sponsors:
  - Core simulation: DOE-NE (NEERs, NERIs and NEUPs), INL (collaborating lab), CNSC (CANDU)
  - Detector simulation, (e, γ) transport: DOE-NNSA
  - Radiotherapy simulation: GCC (proof of concept)
- Other:
  - The presenting author (F. Rahnema) owns equity in a company that has licensed the COMET technologies from Georgia Tech. This study which is a demonstration of COMET could affect his personal financial status. The terms of this arrangement have been reviewed and approved by Georgia Tech in accordance with its conflict of interest policies.

Current tools in use by Georgia Tech for AHTR analysis

Bojan Petrovic (GT)

Tools Used at Georgia Tech for FHR Analysis

Bojan Petrovic (Georgia Tech)

Workshop on Tools for Modeling and Simulation of Fluoride Cooled High Temperature Reactors (FHR)

Georgia Institute of Technology, Atlanta, GA

March 8-9, 2017

Georgia Institute of Technology

Tools (Code Packages) Used at GT for FHR Analysis

FHR-related research

- From ~2009

FHR Analyses

- MS and PhD research (from 2010)
- Senior Design projects (from 2011) – FHR and MSR
- Proposals ……
- NEUP project 2012-2015
- NEUP IRP project 2015-2018

→ Successfully performed/performing analyses of FHR

However:

These were research studies to gain insight into various aspects of FHRs (and MSRs), not design/licensing-level analyses. (Trends are important, simplifications are typically acceptable.)

For academic studies, improved accuracy and efficiency desirable.

For development/design/licensing/deployment: this is critical

Tools (Code Packages) Used at GT for FHR Analysis

Focus on AHTR family of designs (plate fuel)
Some MSR/MSFR Senior Design projects

Core Physics

- SCALE
- SERPENT
- MCNP

Thermal-hydraulics

- RELAP5-3D
- (TRACE)
- Fluent

Materials

Theses related to FHR

Master theses – title or topic

- E. Gros, Liquid Salt Cooled Reactor Start-Up with Natural Circulation under Loss of Offsite Power (LOOP) Conditions
- P. Avigni, Thermal-hydraulic analysis of liquid salt cooled reactors
- S. Lewis, Simplified Core Physics and Fuel Cycle Cost Model for Preliminary Evaluation of LSCR Fueling Options
- C. Kingsbury, Fuel Cycle Cost and Fabrication Model for Fluoride-Salt High-Temperature Reactor (FHR) "Plank" Fuel Design Optimization
- P. Burke, MSRE benchmark
- H. Noorani, MSRE benchmark

PhD dissertations – title or topic

- L. Huang, Investigation of Fuel Cycle of Liquid Salt Cooled Reactors
- K. Ramey, Implementing T/H feedback capability in SERPENT
- P. Avigni, Thermal-hydraulic and safety analyses for on-line refueling of liquid-salt cooled reactors
- T. Flaspoehler, Efficient hybrid transport methodology for shielding analyses (applied to several reactor types, including FHR)

Senior Design Projects Related to FHRs and MSRs

15 Senior Design Projects (2010-2017)

Funded Projects

- NEUP 2012-2015: Fuel and Core Design Options to Overcome the Heavy Metal Loading Limit and Improve Performance and Safety of Liquid Salt Cooled Reactors

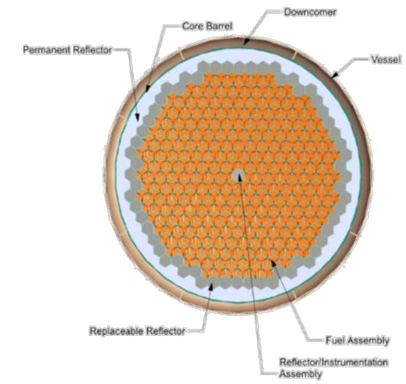
- NEUP IRP 2015-2018: Integrated Approach to Fluoride High Temperature Reactor (FHR) Technology

Core Physics Tools Used at GT for FHR Analysis

Applied to analyze AHTR and MSR designs

- SCALE
- SERPENT
- MCNP

Core Physics Tools Used at GT for FHR Analysis SCALE

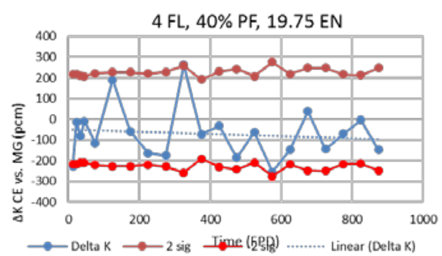


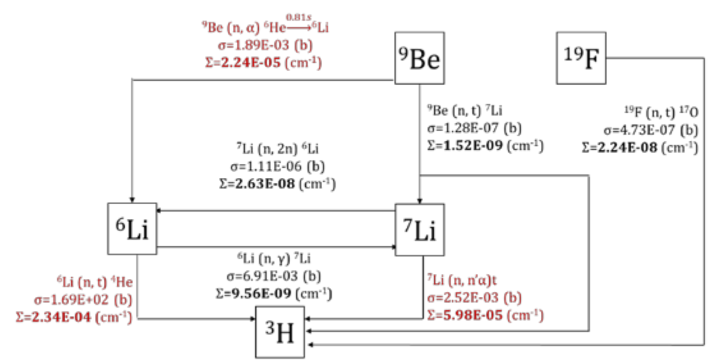
Applications

- AHTR fuel cycle study
- FHR designs for a range of applications
- Online (on-power) refueling
- MSR/MSFR (senior design)

Analyses

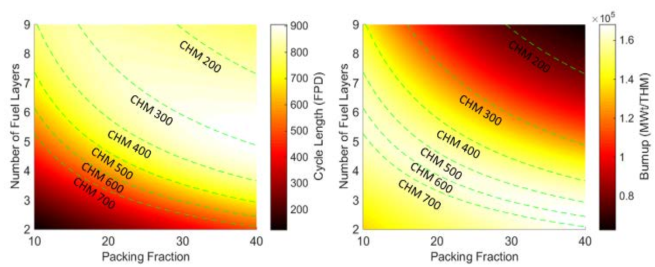
- Assembly and full core
- 2D and 3D
- MG and CE
- Depletion
- Tritium generation

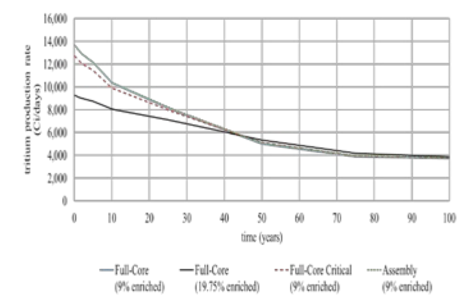




Representative challenges

- Double heterogeneity
- CE vs MG
- (Very) long run time

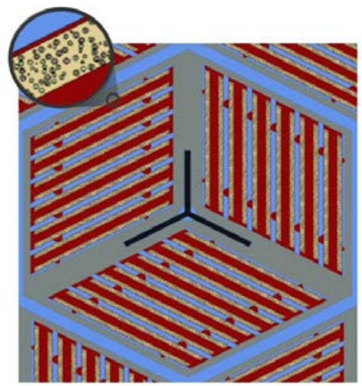




Core Physics Tools Used at GT for FHR Analysis SERPENT (Joint GT&UTK NEUP, most work at UTK)

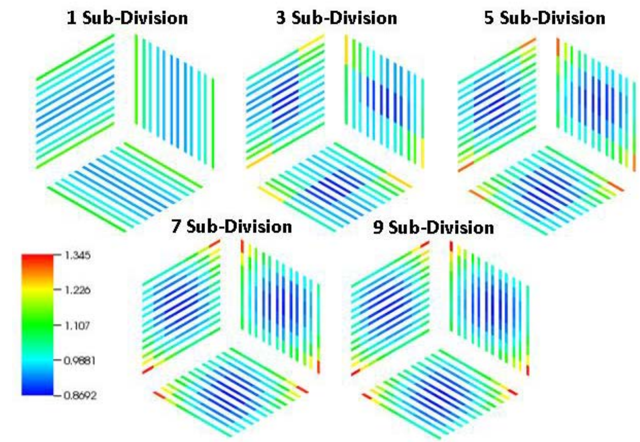
Applications

- AHTR fuel cycle study (at UTK, joint NEUP)
- AHTR analysis



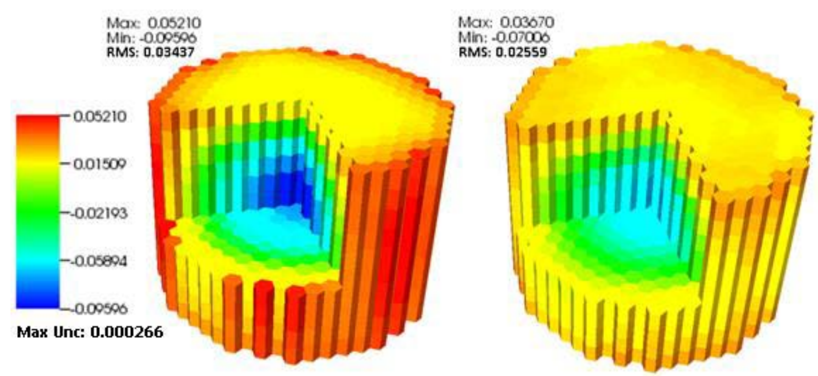
Analyses

- Assembly and full core
- 2D and 3D
- Depletion
- Randomized fuel particles
- 2-step
- (working on) Core depletion with T/H feedback



Representative challenges

- Run time
- Lack of T/H feedback
- …….



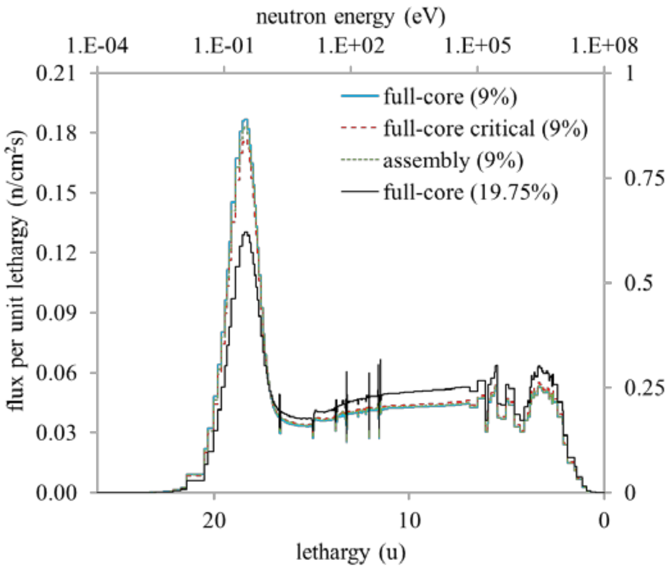
Core Physics Tools Used at GT for FHR Analysis MCNP

Applications

- AHTR
- Benchmarks, V&V
- Tritium generation

Analyses

- Assembly and full core
- 2D and 3D
- Depletion



Representative challenges

- Run time
- Detailed tallies – run time
- Source convergence (global tilt), typical for MC codes
- Lack of T/H feedback
- …….

Thermal-Hydraulics Tools Used at GT for FHR Analysis

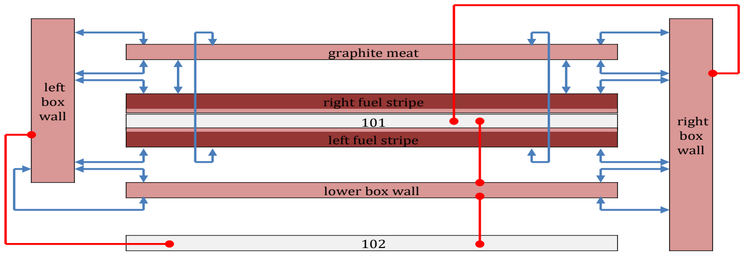
Applied to analyze AHTR designs

- RELAP5-3D
- (TRACE – at ORNL)
- Fluent

Thermal-Hydraulics Tools Used at GT for FHR Analysis RELAP5-3D

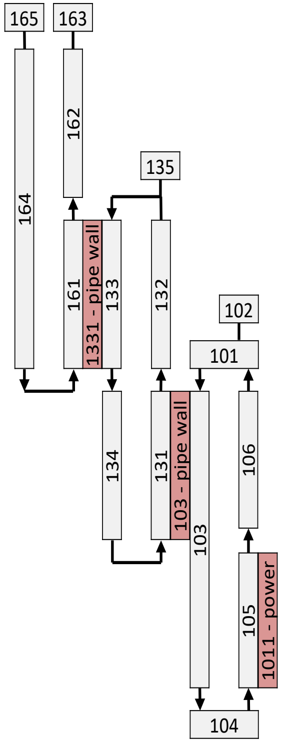
Applications

- Bootstrap under LOOP
- DRACS performance
- LOFC
- Online refueling
- ……



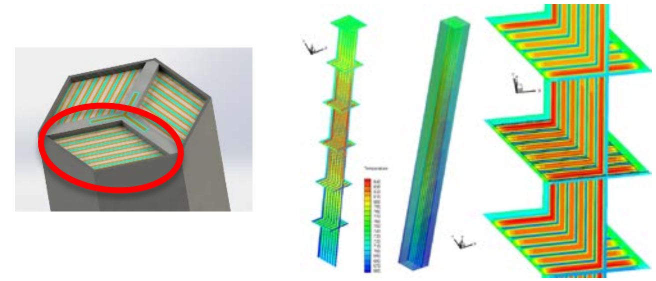
Representative challenges

- How to represent fuel assembly?
- Uncertainties in salt properties
- Need experiments & CFD to generate parameters/correlations
- Integration
- …

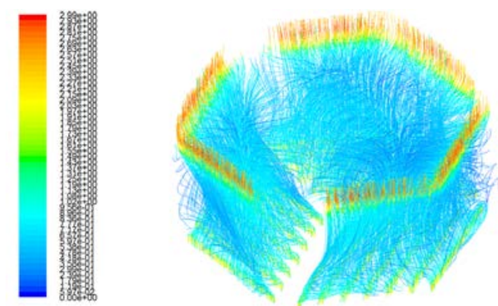


Thermal-Hydraulics Tools Used at GT for FHR Analysis FLUENT

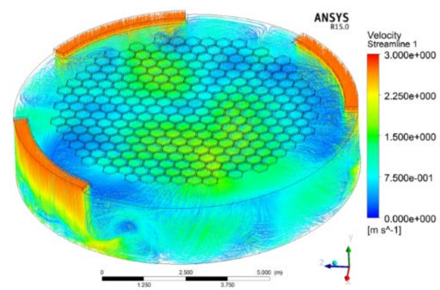
1/3 Fuel assembly thermal distribution:
- Evaluate thermal peaking factors
- Optimize fuel assembly design for heat removal



Flow in the channel of the replaced assembly:
- Simulate assembly extraction
- Characterize flow change during removal



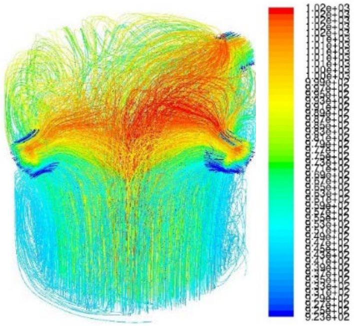
Flow in the lower plenum:
- Simulate flow mixing
- Simulate inlet conditions for core

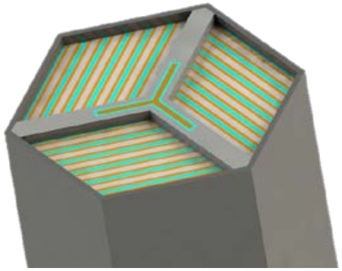


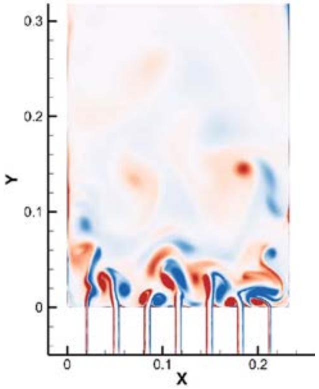
Representative challenges:
- Computationally intense (simulation and visualization
- Coupling to system codes, neutronics, materials/fuel performance
- Need for scaled experiments for validation

Thermal-Hydraulics Tools Used at GT for FHR Analysis
Proposed benchmarks for V&V

Flow distribution in the upper plenum
- Large computational domain
- Affects maximum allowed alloy temperature





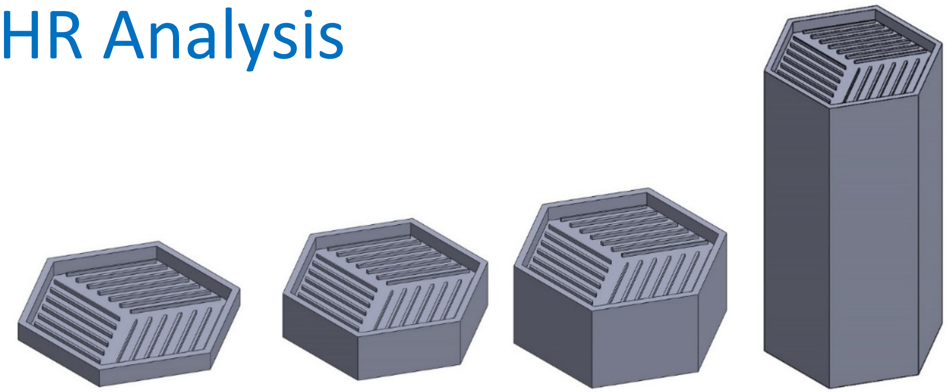


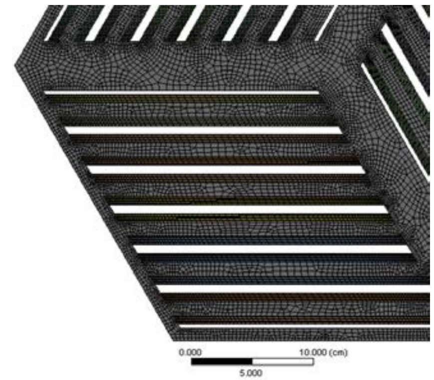
Flow distribution at assembly level
- Characterization of vorticity interactions at channel outlets
- Affects assembly temperature and flow mixing

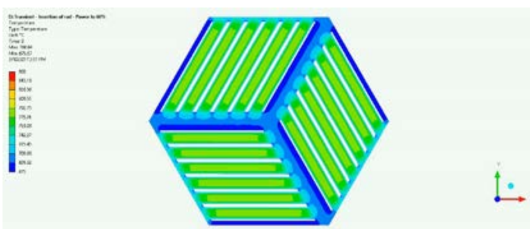
LOOP transient modeling (TRACE/RELAP)
- Integral AHTR system modeling
- Evaluate system response in accidental conditions

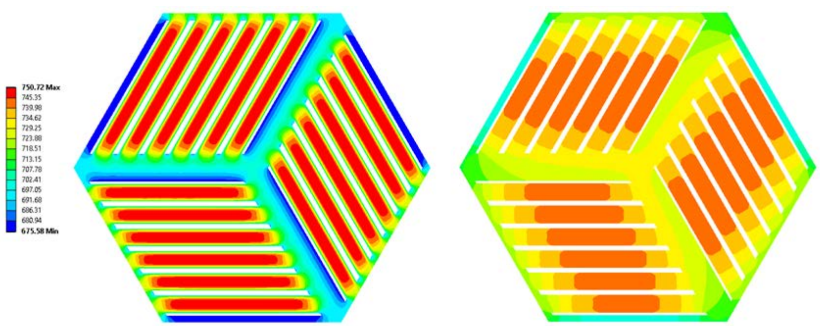
Thermal Analysis at GT for FHR Analysis
ANSYS Mechanical

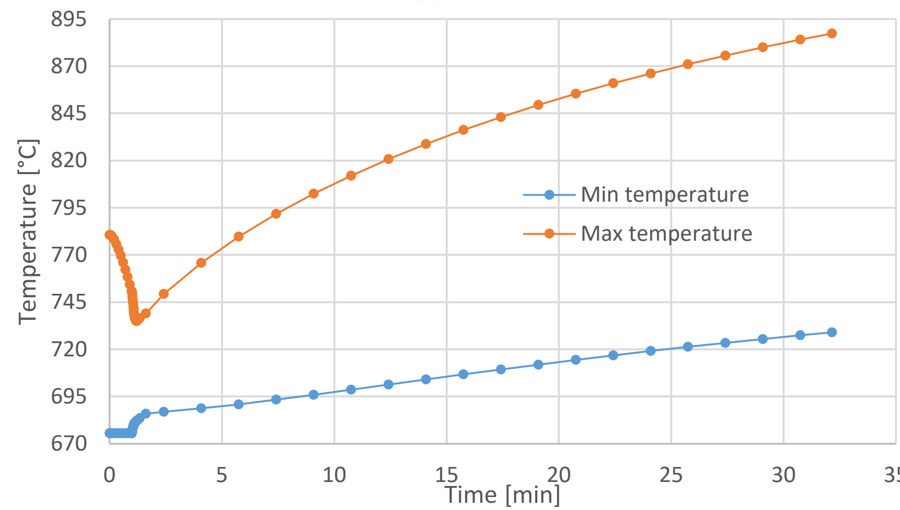
Online (on-power) refueling
Fuel assembly removal
Extraction to argon plenum
Transient temperature?











Conclusions

Performed/performing analyses of FHR at Georgia Tech
Research studies to gain insight into various aspects of FHRs (and MSRs).
Typically, trends are important, simplifications are acceptable.

For future academic studies, improved accuracy and efficiency are desirable.

For design/licensing/deployment these improvements are necessary/critical:

- Integration, practicality o use (→ Workbench)
- Accuracy
- Efficiency
- Adding missing features
- Technical “details”
- …….

Thank you for your attention!

Questions?

Current tools in use by UCB for PB-FHR analysis

Max Fratoni (UCB) – ***Slides unavailable***

Issues with modeling and simulation of tritium management in salt system

Pattrick Calderoni (INL)

Issues with modeling and simulation of tritium management in salt systems

March 8-9, 2017

Georgia Institute of Technology

Pattrick Calderoni

Group lead – Advanced instrumentation development

www.inl.gov

Idaho National Laboratory

Outline

Tritium transport modelin g	TRIDENT analysis (J. Stempien Ph.D. work at MIT)
V&V	T2 experiments at STAR (2001-2007) Current experimental capabilities at INL Molten salt instrumentation development

Idaho National Laboratory

Workshop on Tritium Control and Capture in Salt-Cooled Fission and Fusion Reactors:

Experiments, Models and Benchmarking

October 27-28, 2015
Salt Lake City, UT

Contact: David Carpenter (david_c@mit.edu)

NUCLEAR TECHNOLOGY · VOLUME 197 · 000–000 · FEBRUARY 2017

DOI: http://dx.doi.org/10.13182/NT16-101

ANS

Critical Review

Tritium Control and Capture in Salt-Cooled Fission and Fusion Reactors: Status, Challenges, and Path Forward

Charles W. Forsberg,[a*] Stephen Lam,[a] David M. Carpenter,[b] Dennis G. Whyte,[c] Raluca Scarlat,[d] Cristian Contescu,[e] Liu Wei,[f] John Stempien,[g] and Edward Blandford[h]

NSE
Nuclear Science & Engineering at MIT
science : systems : society

MIT NUCLEAR REACTOR LABORATORY
AN MIT INTERDEPARTMENTAL CENTER

PSFC
MIT Plasma Science & Fusion Center

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Tritium Transport and Corrosion Modeling in the Fluoride Salt-Cooled High-Temperature Reactor

John D. Stempien, PhD

Content Based on Doctoral Thesis Defense

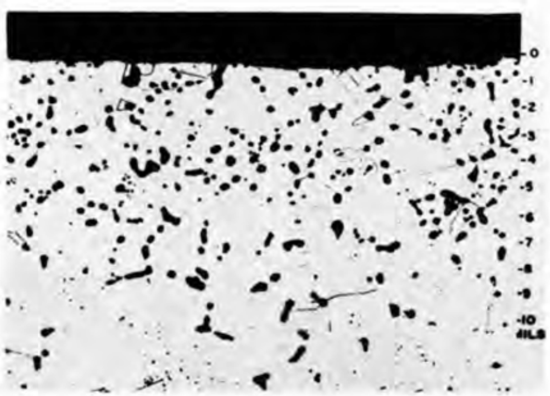
FHR

Massachusetts Institute of Technology

NSE Nuclear Science and Engineering

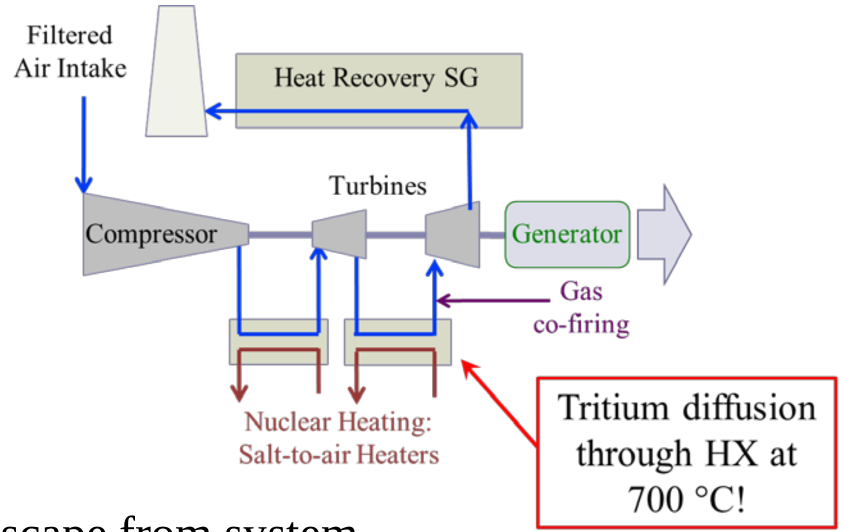
Tritium Poses Two Problems

1. Corrosion - preferential attack of Cr in alloys by TF:
   - $2TF_{(d)} + Cr_{(s)} \rightarrow CrF_{2(d)} + T_{2(g)}$
   - Corrosion reaction consumes TF, generates T_2



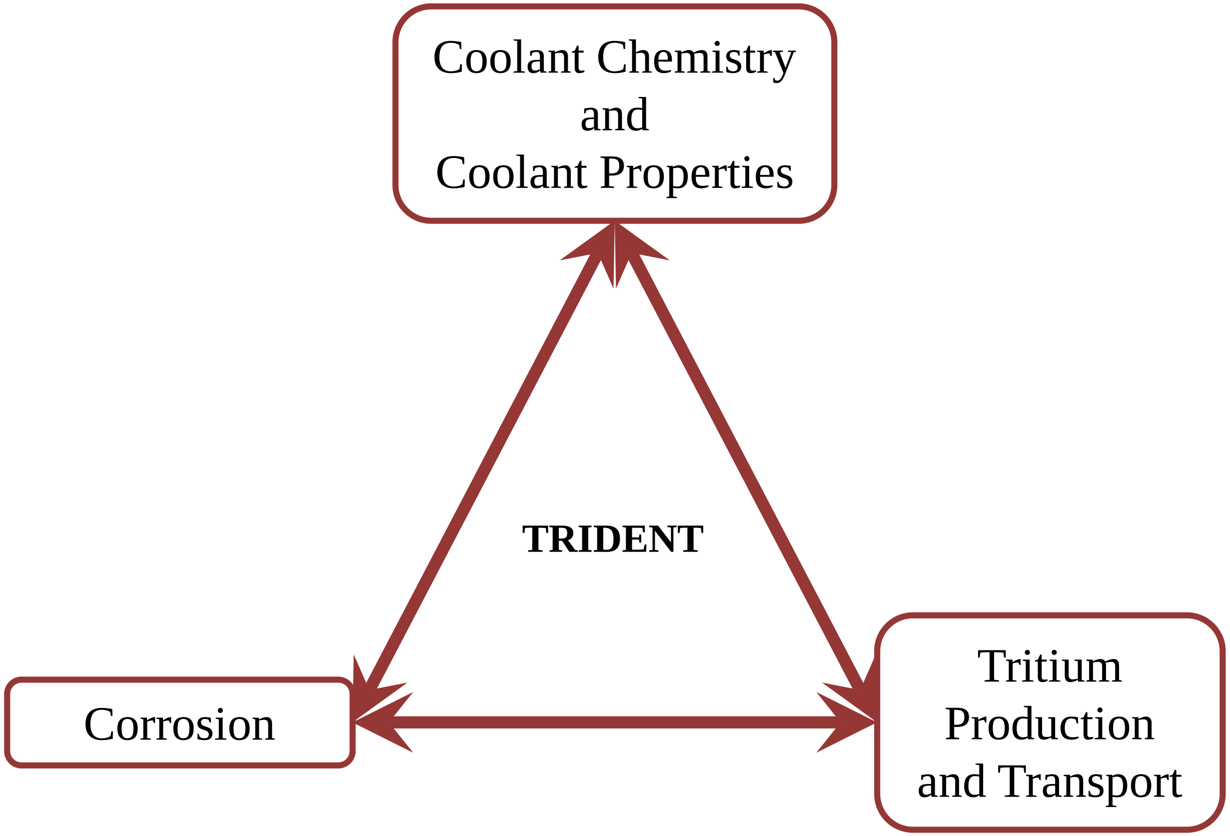
Pitting in Inconel exposed to fluoride salt high in HF (Image from ORNL-2349)

2. Radiological:
   - T_2 fast diffusion through metal
   - $T_{1/2}$ = 12.3 yr
   - β = 5.9 keV



- Must control corrosion and manage tritium escape from system
- Modeling/simulation to help evaluate tritium control options

TRIDENT (TRItium Diffusion EvolutioN and Transport) Was Developed to Link FHR Tritium Behavior to Coolant Chemistry



Basic Elements of TRIDENT:
Tritium Generation in Flibe Coolant

Neutron Transmutation Generates Tritium in Flibe

$$^{6}LiF + n \rightarrow He + TF$$

$$^{7}LiF + n \rightarrow He + TF + n'$$

$$BeF_2 + n \rightarrow {}^{4}_{2}He + {}^{6}_{2}He + 2F^{-}$$

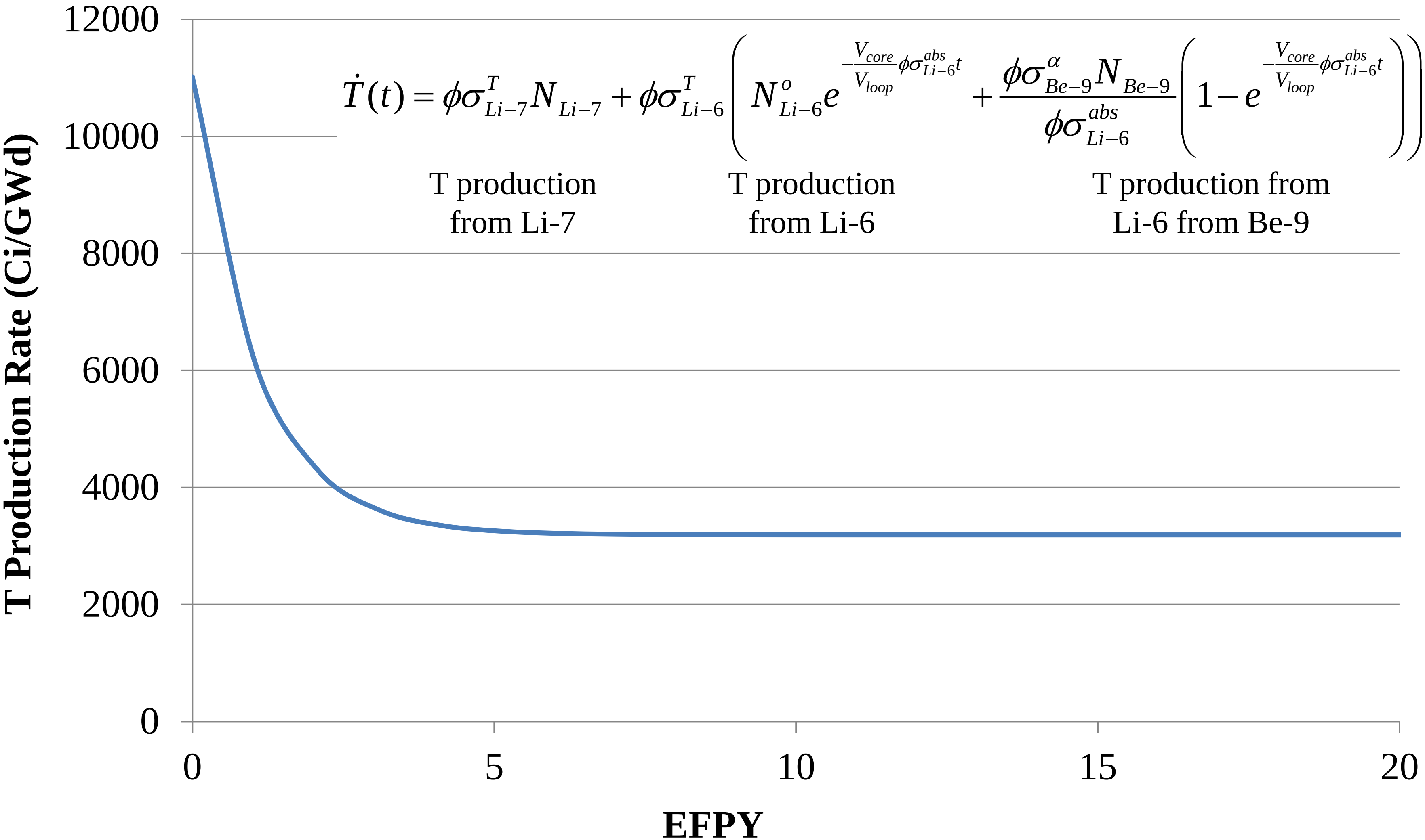
$$^{6}_{2}He \rightarrow \underbrace{^{6}_{3}Li} + e^{+} + \bar{\nu}_e \quad (t_{1/2} = 0.8 \text{ sec})$$

^{6}Li = 0.005 wt%

^{7}Li = 99.995 wt%

	One-group Cross section (b)
$\sigma^{T}_{Li\text{-}6}$	148
$\sigma^{\alpha}_{Be\text{-}9}$	3.63×10^{-3}
$\sigma^{T}_{Li\text{-}7}$	1.00×10^{-3}

FHR Tritium Production Rate is Not Constant



$$\dot{T}(t) = \phi\sigma^{T}_{Li-7}N_{Li-7} + \phi\sigma^{T}_{Li-6}\left(N^{o}_{Li-6}e^{-\frac{V_{core}}{V_{loop}}\phi\sigma^{abs}_{Li-6}t} + \frac{\phi\sigma^{\alpha}_{Be-9}N_{Be-9}}{\phi\sigma^{abs}_{Li-6}}\left(1-e^{-\frac{V_{core}}{V_{loop}}\phi\sigma^{abs}_{Li-6}t}\right)\right)$$

T production from Li-7

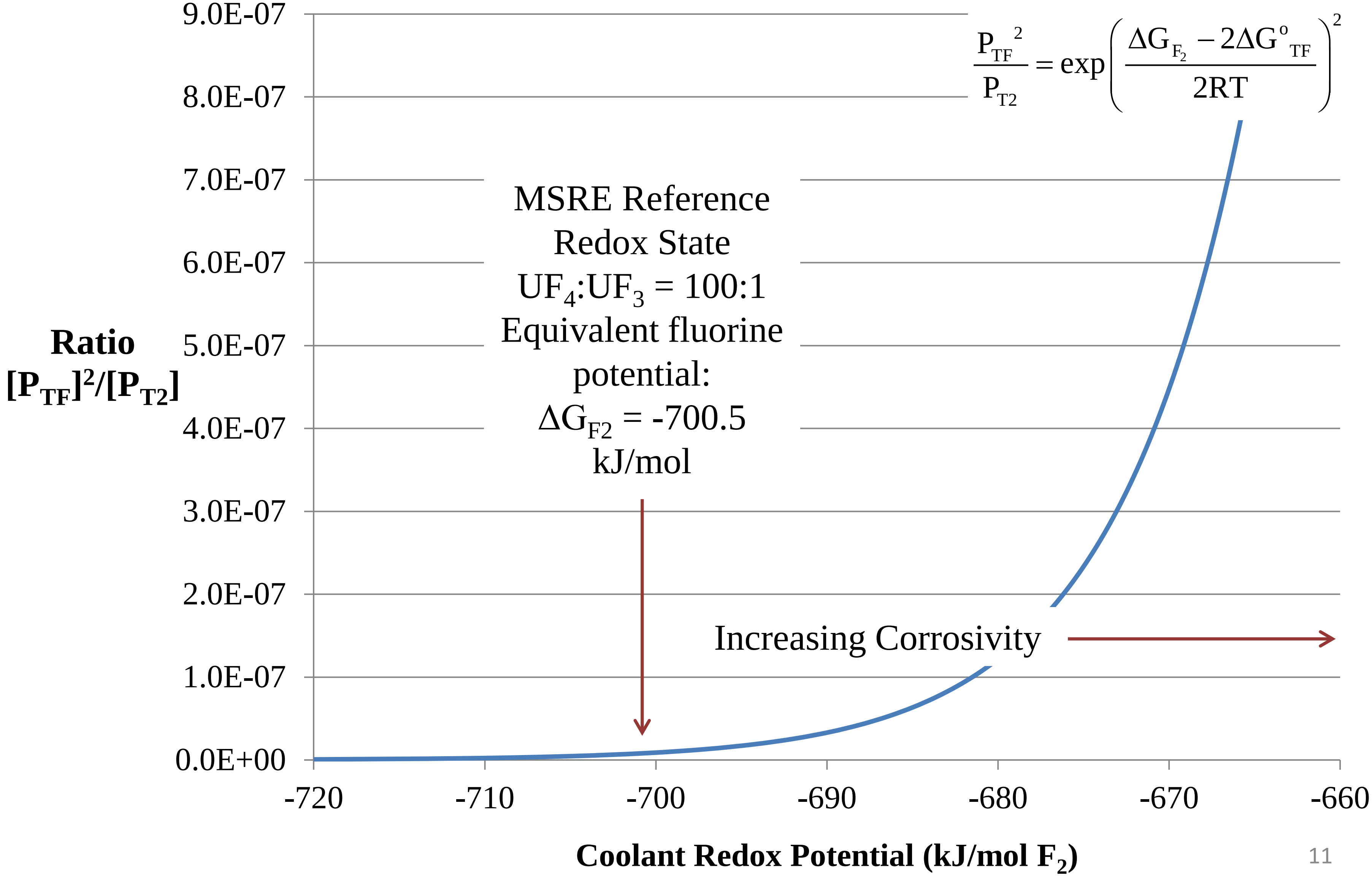
T production from Li-6

T production from Li-6 from Be-9

Note: Plot was made for Mk1 PB-FHR. Energy-averaged flux and cross sections vary with reactor. Time to reach equilibrium T production rate also varies with relative volumes of salt in the reactor core versus salt filling the rest of the system.

Basic Elements of TRIDENT:
Effect of Redox on Corrosion and Tritium Behavior

Redox Potential Dictates Relative Amounts of T_2 and TF



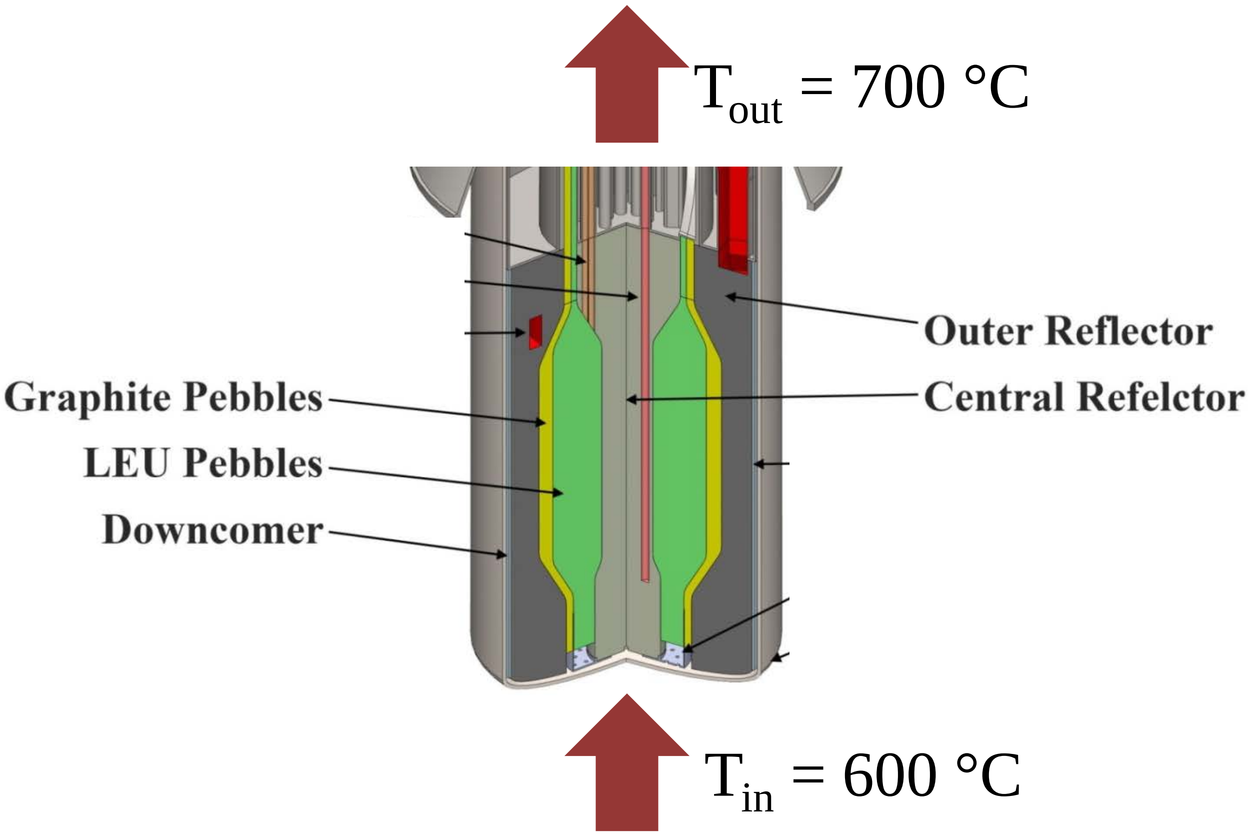
TRIDENT Tritium Diffusion and Corrosion Models Were Benchmarked Against Experiments

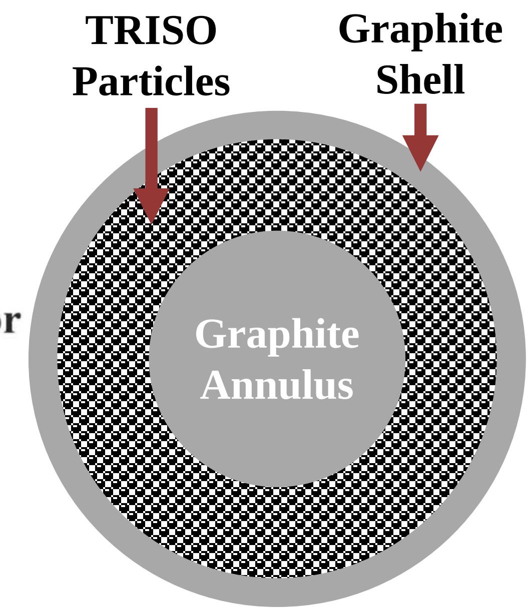
- Tritium diffusion in Nickel/Flibe and Nickel/Flinak systems
  - Experiment: FUKADA, S., MORISAKI, A., "Hydrogen permeability through a mixed molten salt of LiF, NaF and KF (Flinak) as a heat-transfer fluid," *Journal of Nuclear Materials*. **358**, 235–242 (2006).
  - Experiment: CALDERONI, P., SHARPE, P., HARA, M., OYA, Y., "Measurement of tritium permeation in flibe (2LiF–BeF2)," *Fusion Engineering and Design*. **83**, 1331–1334 (2008).

- Corrosion and corrosion product mass transfer in flibe containing dissolved UF_3/UF_4
  - Experiment: KEISER, J.R., "Compatibility Studies of Potential Molten-Salt Breeder Reactor Materials in Molten Fluoride Salts," ORNL/TM-5783, Oak Ridge National Laboratory, (1977).

Modeling Tritium Behavior in the FHR: TRIDENT Code Description

Results of TRIDENT Simulations of Baseline 236 MWt Mk1 PB-FHR





FHR Release Rate Without Tritium Capture is High

- FHR tritium release rate with no engineered tritium mitigation systems:

~ 2500 Ci/EFPD for 236 MWt PB-FHR (10600 Ci/GWD)

- HWR tritium release rate:

20 Ci/GWD

- LWR tritium release rate:

< 1 Ci/GWD

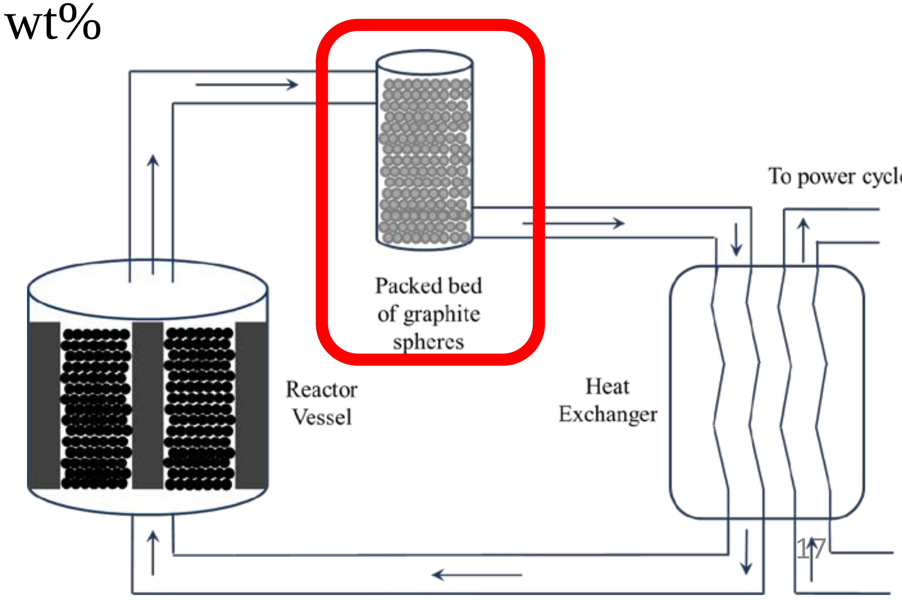
TRIDENT Simulations of Proposed Tritium Mitigation Methods

- Permeation windows
- Counter-current gas stripping
- Capture on graphite outside of core
- Tungsten (or other coating) in heat exchanger
- Increased Li-7 enrichment in flibe

Conclusions on Tritium and Corrosion

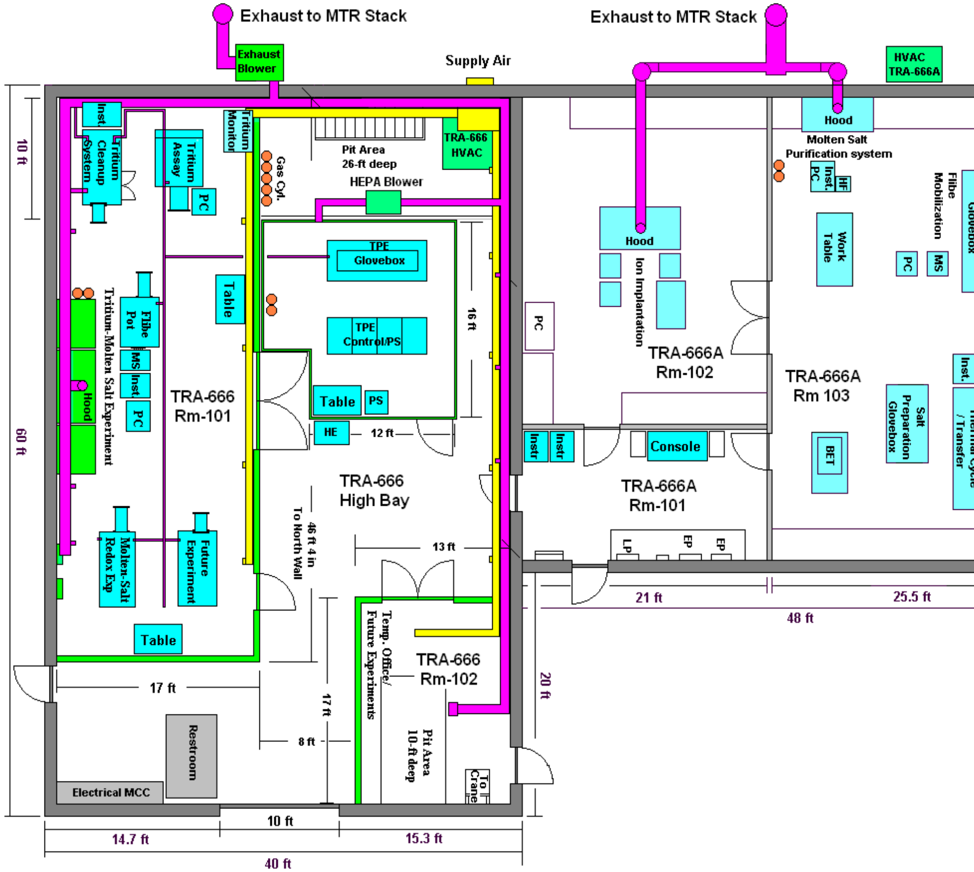
Simulations show:

- Corrosion rate with controlled redox: 0.08 mg/cm^2 per EFPY
- Tritium release rates without engineered solutions: 2500 Ci/d
- Proposed New Solutions:
  - Sorption on bed of graphite release rates < 10 Ci/EFPD
  - Increase Li-7 enrichment to 99.999 wt%
  - Use of W permeation barrier



Selected Future Work

- Wide option space for tritium control, need to optimize size/performance of capture systems
- Explore use of graphite specifically engineered for tritium capture (outside of core)
- May include radiation effects on graphite for tritium absorption in core
- Model tritium/protium isotopic exchange reactions if H_2 deliberately added to system
- Improve corrosion model: currently modeled as 1D grain boundaries not as 3D networks
- Need for experimental work:
  - Tritium transport in flowing salt contacting metal membranes and graphite
  - Tritium uptake and desorption kinetics on graphite in salt over range of temperatures, at low partial pressures of T, and on relevant grades of graphite
  - Must know redox state of all salt experiments



T2 experiments at the INL Safety and Tritium Applied Research (STAR) facility (2001-2007)

Overview of JUPITER-II program (Apr. 2001 – Mar. 2007)

- JUPITER-II
  - **J**apan-**U**SA **P**rogram of **I**rradiation/**I**ntegration **Te**st for Fusion **R**esearch –**II**
  - Six years (2001-2006) under the collaboration implemented between MEXT (Ministry of Education, Culture, Sports, Science and Technology) and US DOE
- Task 1: Self-cooled liquid blanket
- **Task 1-1: FLiBe system**
- (Task 1-1-A) FLiBe Handling/Tritium Chemistry
  - Experimental work with FLiBe at STAR, INL for self-cooled liquid blanket of a fusion reactor.
  - Maintaining Flibe under a reducing atmosphere is a key issue to transform TF to T_2 with a faster reaction rate compared with the residence time in blanket.
  - The purpose of the task is to clarify whether or not the Redox control of Flibe can be achieved with Be through the following reaction.
    - $Be + 2\ TF \rightarrow BeF_2 + T_2$
- (Task 1-1-B) FLiBe Thermofluid Flow Simulation
  - Simulation work at U. of Kyoto and UCLA

Reference:

K. Abe, A. Kohyama, S. Tanaka, T. Muroga, C. Namba, S.J. Zinkle, and D.K. Sze "Summary Report of Japan-US Joint Project (JUPITER-II)" *NIFS- PROC-71 (2008)*

JUPITER-II (2001-2006)
Task 1-1-A: FLiBe Chemistry Control, Corrosion, and Tritium Behavior

- **Mobilization studies**
  - Developed and Validated Transpiration System for Vapor Pressure Measurement of Molten Salts
  - Measured FLiBe Vapor Pressure at Low-temperature range Relevant to Fusion Blanket Designs
  - **Experimental procedure:**
    - Mobilization test was performed with Ar, air, and moist air in inert gas glove box.
    - (Ar test) conducted at 500, 600, 700, and 800°C with 25 sccm Ar flow
    - (Air test) conducted at 500, 600, 700, and 800°C with 25 and 50 sccm air flow
    - (Moist air test) conducted at 600, 700, and 800°C with 25 and 50 sccm moist air flow
    - Both Ni and glassy carbon crucibles were used

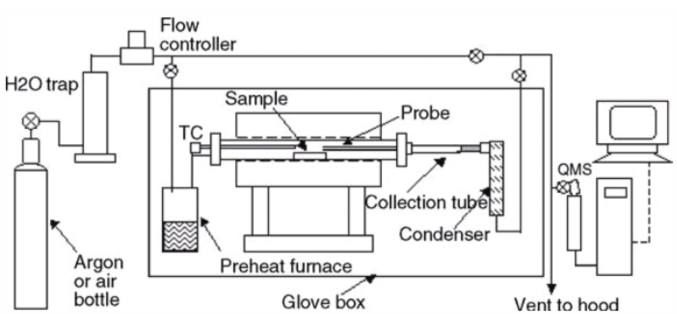


Fig. 1. Transpiration test setup.

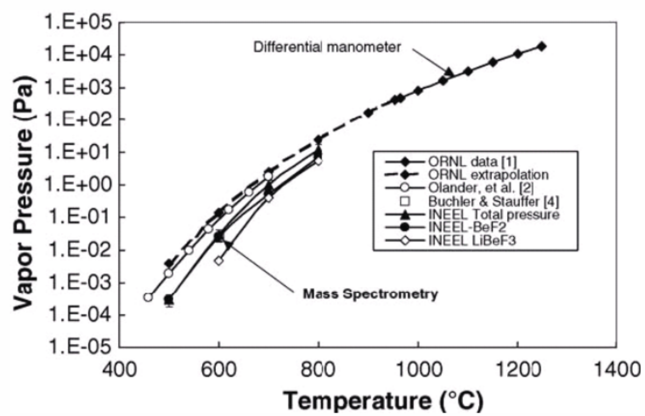


Fig. 2. Total pressure over Flibe.

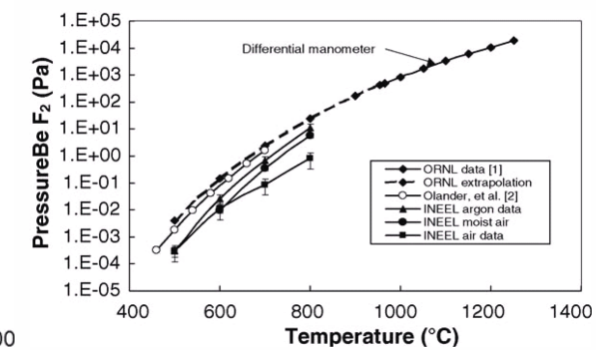


Fig. 3. BeF_2 pressure in various environments.

JUPITER-II (2001-2006)
Task 1-1-A: FLiBe Chemistry Control, Corrosion, and Tritium Behavior

- **Redox control**
  - Demonstrated active control of the fluorine potential in FLiBe/Nickel systems using metallic Be
  - Proved the inhibition of FLiBe corrosion of Reduced Activation Ferritic Steel in static conditions
  - **Experimental procedure:**
    - The purpose of the task is to clarify whether or not the Redox control of Flibe can be achieved with Be through the Be + 2 TF ➔ $BeF_2 + T_2$ reaction
    - HF was bubbled with He and H_2 through FLiBe with various concentration of dissolved Be (cylindrical Be rod, 0.76 cm OD and 3 cm long) .
    - Ni crucible and Ni tubes were used and all the wet surface was Ni coated

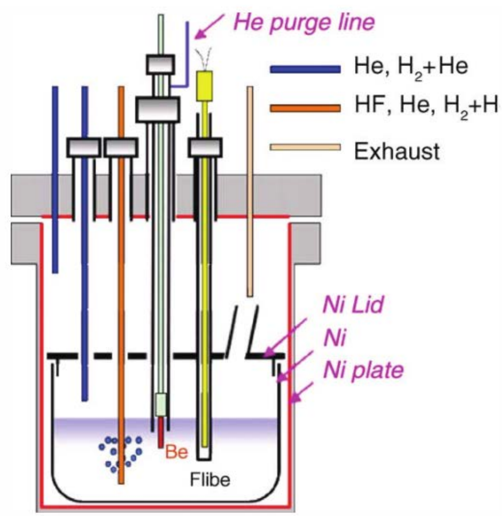


Fig. 5. Reactor for measuring redox

RAFS sample and metallic Be rods used for Redox and corrosion tests before and after immersion in FLiBe bath

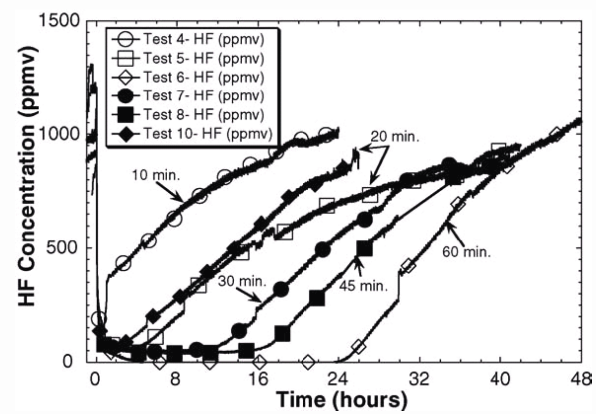


Fig. 6. HF concentration measured by QMS on the outlet of the REDOX experiment for several Be immersion times.

JUPITER-II (2001-2006)

Task 1-1-A: FLiBe Chemistry Control, Corrosion, and Tritium Behavior

- **D_2 and T_2 permeation**
  - Measured transport properties (diffusivity and solubility) of D_2 and T_2 in FLiBe between 550 and 700 C
  - Investigated the effect of FLiBe Redox condition on T_2 transport
  - **Experimental procedure:**
    - (D_2 test) was conducted in a cylindrically symmetric dual probe permeation pot
      - Ni crucible and Ni tubes are used
      - at 600 and 650°C at 9.0×10^4 Pa in NI Probe 1
    - (T_2 test) was conducted in a permeation pot with 2mm thick Ni membrane
    - at 550, 600, 700 and 800°C with 1 and 20 sccm (0.1 ppm-10 vo..% T_2/Ar)
    - Measured with QMS and GC

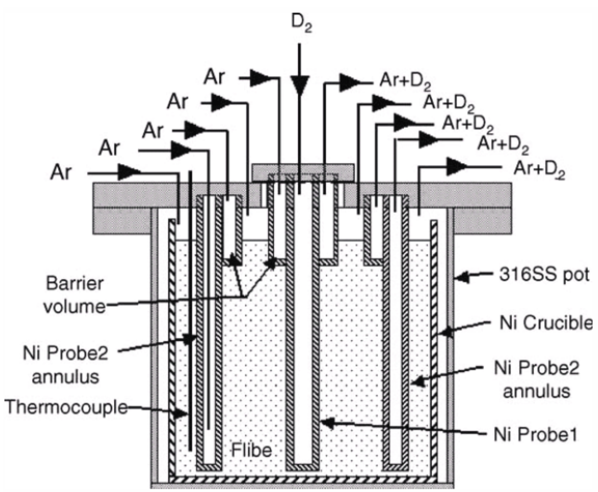


Fig. 10. Schematic illustration of cylindrically symmetric, permeation probe assembly.

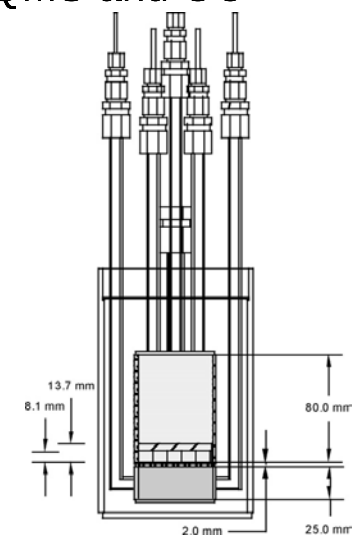


Fig. 1. Permeation cell scheme with relevant dimensions.

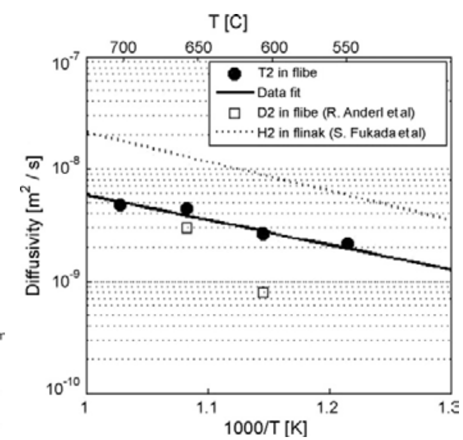


Fig. 3. Measured T diffusivity in flibe.

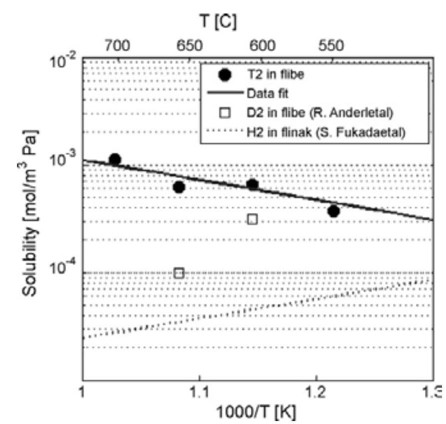


Fig. 4. Measured T solubility in flibe.

INL current experimental capabilities

Fuel cycle technologies

- Material and Fuel Complex (MFC) facilities – cold labs, hot cells
- Chloride salts (Li, Na, U, …): extensive experience with electrochemistry and fuel products characterization

STAR

- Tritium transport modeling and experimental validation
- Flibe properties characterization

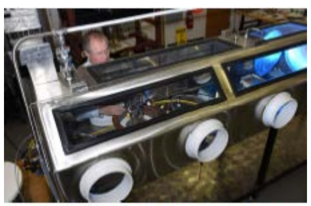
ARTIST facility for thermal-hydraulics codes V&V (planned)

- Multiple forced convection loops with different coolants
- Validation of high temperature flow, heat transfer, and thermal energy storage

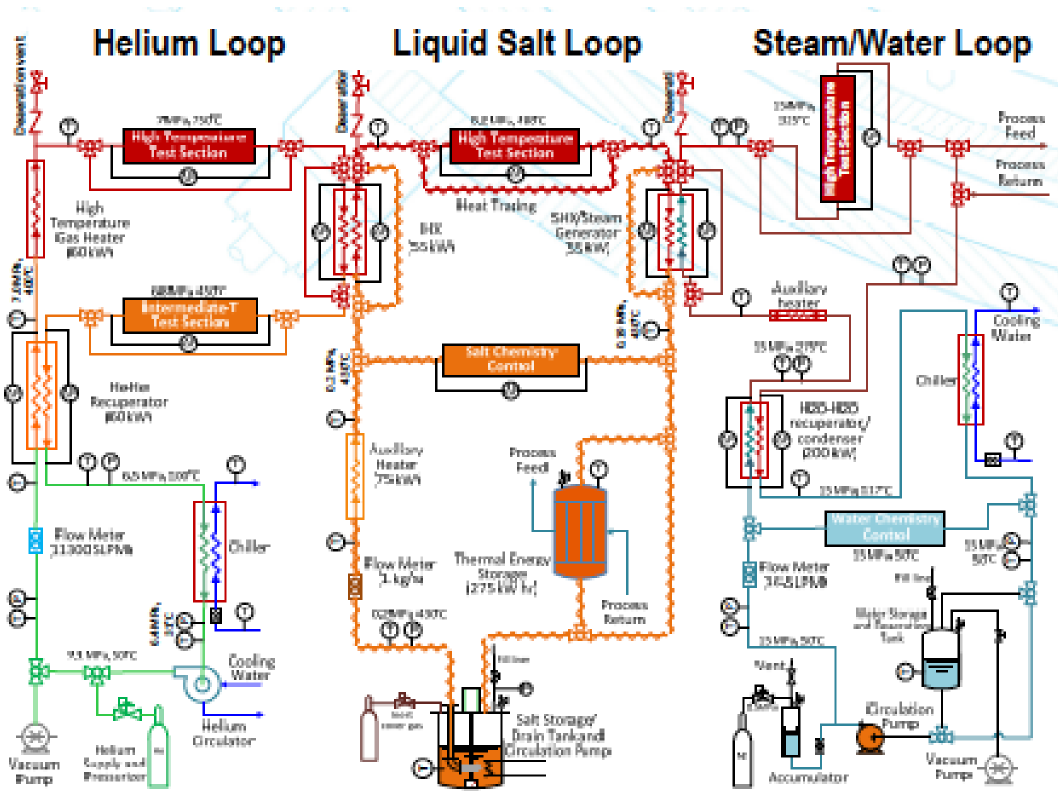
Advanced nuclear instrumentation development program

- High Temperature Test Laboratory (HTTL)

Advanced Reactor Technology Integral System Test (ARTIST) Facility



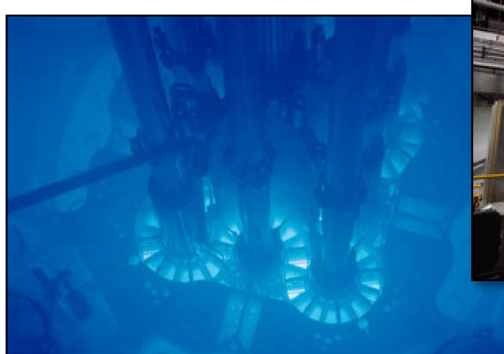
Glove box for salt mixture preparation



Note: The high-pressure hot water loop is now in the final detail design stage. It will be assembled during FY17 with support from NE-HES funding

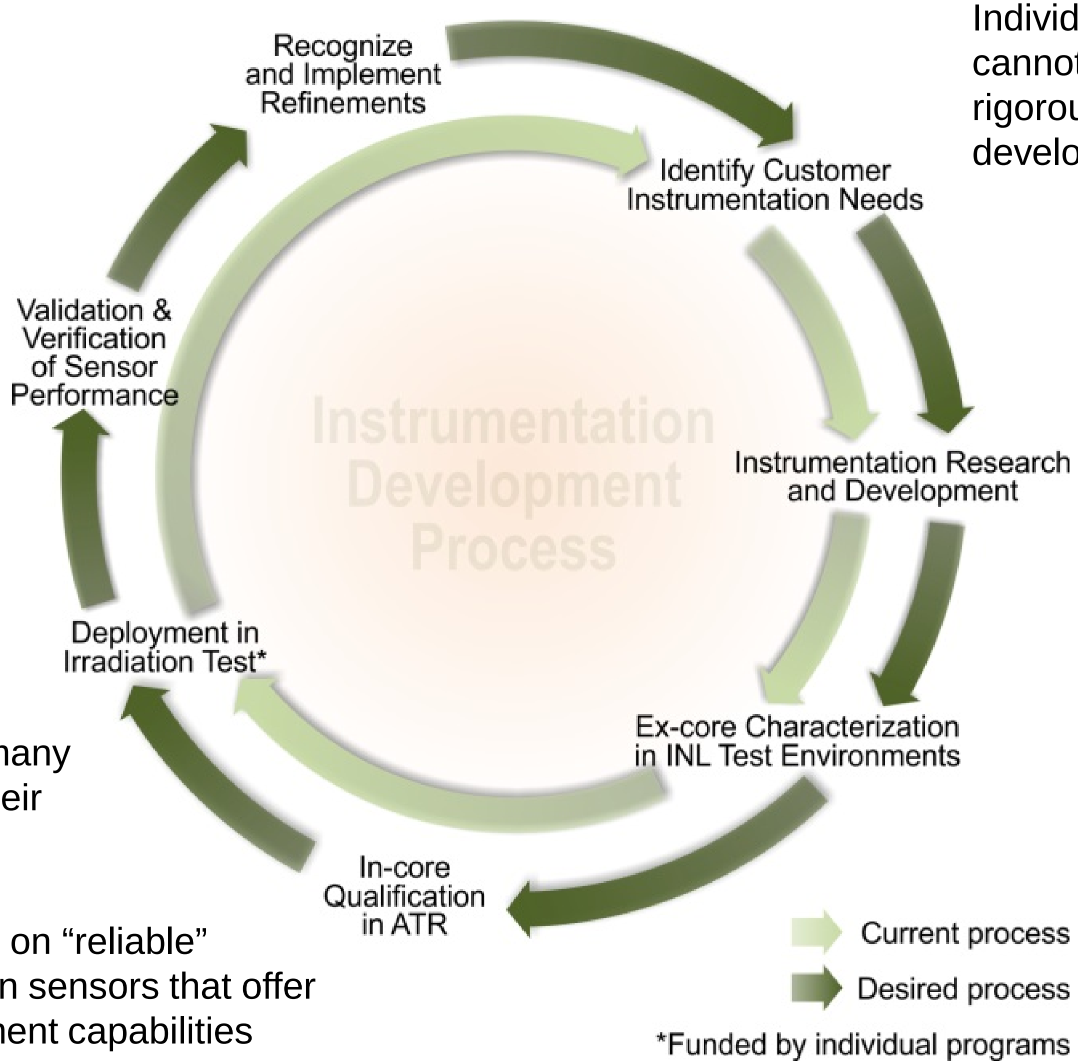
Motivation for Advanced Instrumentation Development

- Advanced fuel and material development requires measurements of material behavior at smaller length and time scales <u>during irradiation</u>
- NE approach combines advanced post-irradiation examination (PIE) with multiscale and multi-physics fuel performance modeling. However, connecting measurements with predictive modeling will require dramatic advances in in-core instrumentation
- Support the GAIN initiative by developing new industry-relevant measurement and data transmission
- Irradiation testing in a material test reactor is a complex and challenging measurement environment:
  - Temperature and pressure extremes
  - Wide power and time scale extremes (TREAT vs. ATR)
  - Radiation effects
  - Feed-through limitations
  - Difficult geometries



Current approach to in-reactor instrumentation development <u>is not working</u>

Individual programs often cannot afford (time & money) rigorous instrumentation development requires



Accelerate deployment

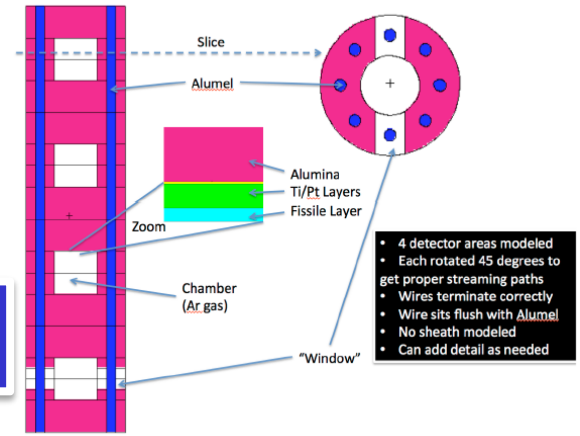
Sufficient in-reactor testing is typically not performed to qualify many instruments prior to their end use:

- premature failure
- continued reliance on “reliable” sensors rather than sensors that offer desired measurement capabilities

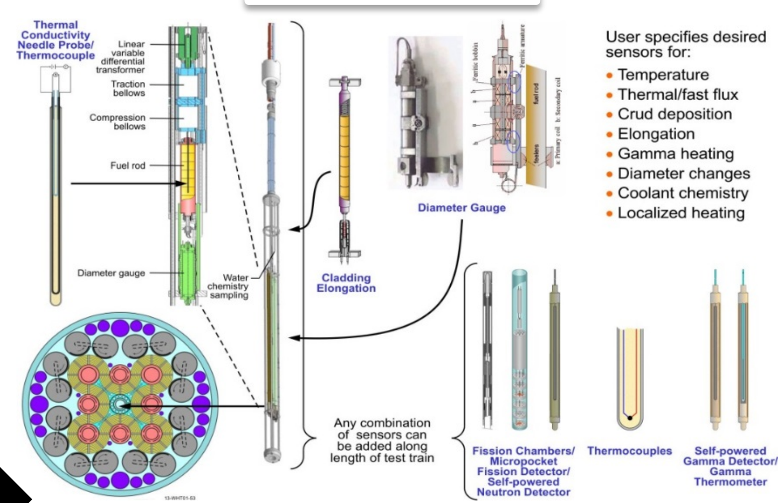
Advanced Instrumentation Vision

- Vision: "Plan for Improving Development of In-Reactor Instrumentation Capability at the Idaho National Laboratory" internal report, August, 2015
  - High-level Requirements
    - Synergistic relationship with Modeling and Simulation
    - Expanded international collaborations
    - Higher-fidelity, real-time data
    - Strategic equipment and personnel investments
- Benefits of INL instrumentation development base capability:
  - Reduced cost for development by leveraging:
    - Personnel expertise
    - Laboratory fabrication and test equipment
    - Test facilities
  - Technology development continuity between program funding interruptions
  - Reduced risk by deploying instruments that have been adequately qualified in-core

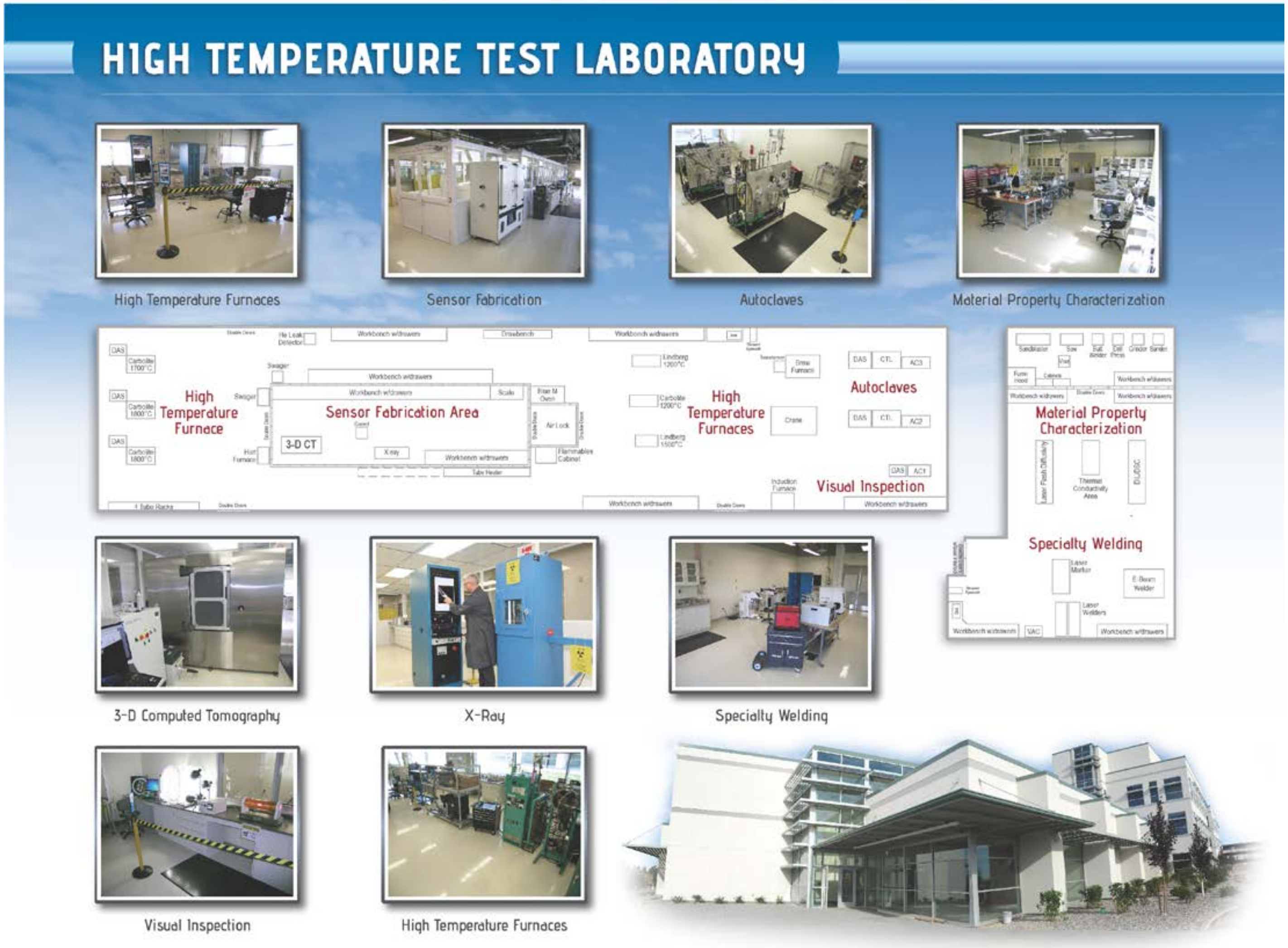
Science-based R&D



Dedicated ATR irradiation



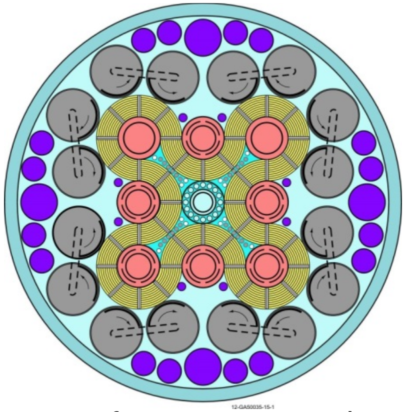
Strategic Investments to Address Mission Goals



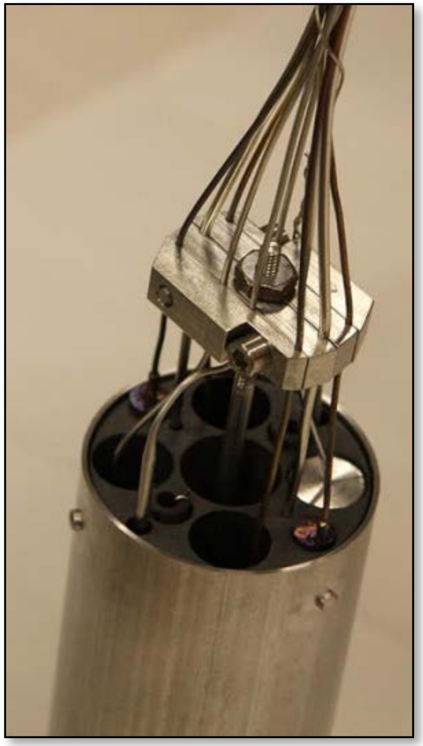
INL's Vision for Evolutionary Advancements

- Near Term (0 – 5 years) Measurements Development
  - Higher Temperatures
  - Miniaturization
  - Radiation Resistance
  - Self Powered
  - Wireless Data Transmission
  - Instrumentation Testing Rig installed in dedicated positions in the ATR and TREAT (MITR and ATF-2 case study)

TREAT instrumented "element" for prototypic transient characterizations



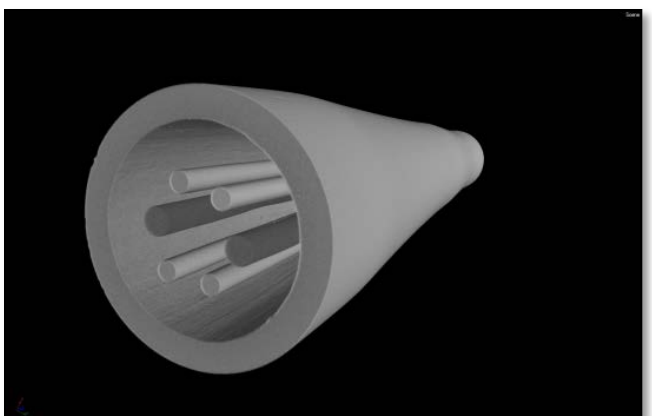
B-11 for near-prototypic steady-state characterizations



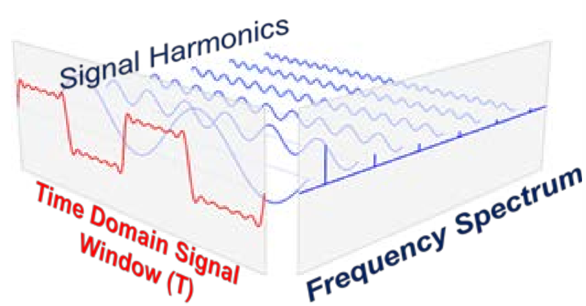
MITR ULTRA Irradiation Test
Flux: MITR << ATR
i.e. irradiation time: MITR >> ATR

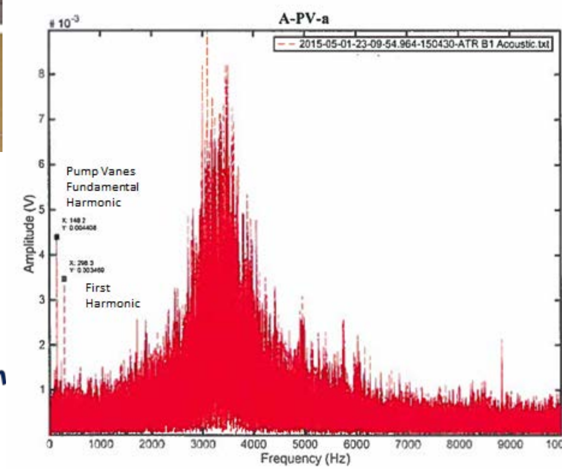
INL's Vision for Revolutionary Advancements

- Long Term (5 – 10 years) Measurements Development
- – Radiation hardened, rapid response for very short duration tests
    - Temperature, gas P and x_i, fuel movement, multiphase coolant regimes
- – Use of Combinatorial Material Science & Modern Manufacturing Technology
    - Screen and optimize sensor materials for sensor design
    - Micro- and Nano-manufacturing techniques
    - 3D Printing and Single Use / Disposable Printed Sensors
    - Embedded sensors integrated in fuels
- Grand Challenge – Measure microstructural changes in-situ and post-irradiation



Images from recently acquired 3-D Computed Tomography Machine

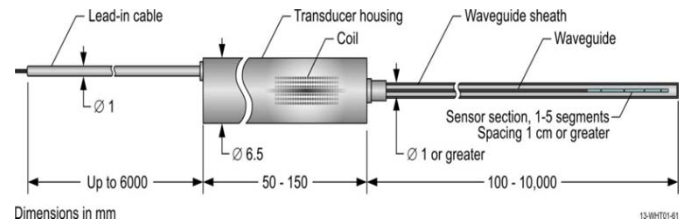


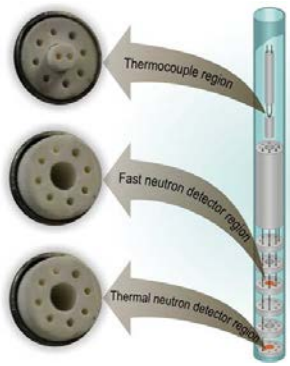


Thermoacoustic Telemeter for in-core sensor transmission

Current Development/Deployment

- Temperature
  - High Temperature Irradiation Resistant (HTIR) TCs (AGR, ATF, TREAT IRP, LDRD*)
  - Ultrasonic Thermometer (Used Fuel Disposition, AGR 5/6/7, ATF)
  - Optical fiber - distributed sensor time domain reflectometry (Rayleigh backscattering) (TREAT IRP, LDRD*)
  - Optical fiber - FBGs (AGR, TREAT IRP, LDRD)
  - Silicon Carbide / Melt wire monitors (ATF, NSUF)
  - Diamond thermistor (TREAT IRP, LDRD*)
  - Optical Pyrometer (ATF)
- Thermal Conductivity
  - Transient Hot Wire Method Needle Probe (TREAT IRP)
- Mechanical response
  - LVDT (LDRD, ATF)
  - Optical fiber – distributed sensor (LDRD*)
  - Acoustic response (LDRD*)
- Neutron Flux
  - Micro-Pocket Fission Detector (NEET, AGR, ATF, TREAT IRP)
  - Self Powered Neutron Detector (ATF)
  - Miniaturized Fission Chambers (NEET)
  - Flux Wires / Foils (NSUF*, LDRD*)
- Crack Growth
  - Direct Current Potential Drop
- Self Powered, Wireless
  - Thermoacoustic response (ATF)
- Void Sensor
  - Boiling Detector (ATF, LDRD*)





Proposed molten salt instrumentation development at INL

- Apply HTTL sensors to molten salt systems requirements
  - Radiation resistant (low drift), reliable (sheet corrosion) Tcs
  - Neutron sensors
  - Optical fiber sensors for temperature and structural health monitoring
  - Ultrasound Thermometry and acoustic response methods

- Electrochemical techniques
  - Optimized electrodes configuration
  - Impedance spectroscopy
  - Rotating disc electrodes

- Spectroscopy
  - Laser Induced Breakdown Spectroscopy (LIBS)

Idaho National Laboratory

The National Nuclear Laboratory